PHASE TRANSITIONS IN LIPID BILAYER MEMBRANES VIA BIFURCATION

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PHASE TRANSITIONS IN LIPID BILAYER MEMBRANES VIA BIFURCATION

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In this work, we use the popular Helfrich-Cahn-Hilliard phase field model for two-component lipid bilayer vesicles to systematically study phase transitions in lipid vesicles. We do this in the context of bifurcation theory.

From a mathematical point-of-view, a particularly troubling aspect of lipid membrane behavior is its fluidity. This manifests as invariance of the energy functional under reparametrizations. The associated symmetry group in this case is the infinite-dimensional diffeomorphism group on S^2. As a consequence, the Euler-Lagrange equations are underdetermined. By viewing this symmetry as an example of a gauge group, we propose a *gauge fixing procedure* using harmonic maps [13] to break the symmetry, thereby removing redundancies from the system.

Applying standard tools of local bifurcation theory to the problem is not straightforward. The $O(3)$ symmetry of the problem renders the linearized Euler-Lagrange equations with a degenerate null space. We use group theoretic strategies [53, 28] to tame this degeneracy and perform a local bifurcation analysis. We establish the existence of local symmetry-breaking branches of solutions bifurcating from a (trivial) spherical homogeneous state. We provide a few explicit examples of these branches in the case of octahedral and icosahedral symmetry using a technique developed by Poole [52].

We computationally study the system for axisymmetric solutions. The gauge fixed formulation is discretized using a Galerkin projection and detailed bifurcation

diagrams are obtained using path-following by systematically exploring the parameter space. We efficiently compute stability of these branches, by employing the block-diagonalization technique using projective operator theory and assemble the hessian in its symmetry adapted basis. The eigen values of the individual blocks are used to assess stability. Explicit expression for the hessian is also presented.

In literature, two possible formulations for the model are available that differ on the nature of the area constraint imposed. Here, we resolve this theoretical dilemma. We prove that lipid membranes of genus zero (homeomorphic to a sphere) can be modelled either as locally or globally area preserving by showing that the two formulations are equivalent with respect to determining equilibrium solutions and their stability.

BIOGRAPHICAL SKETCH

Sanjay Dharmavaram was born in Hyderabad, India. Since it has been such a long time ago, he does not have any recollection of how the first seventeen years passed; except for a vague memory of panicking before Hindi exams and asking his sister for help. After graduating from high school, he moved to Kharagpur, a small town close to Calcutta, for his undergraduate studies at the Indian Institute of Technology, Kharagpur. In 2005, he moved to Ithaca, straight out of college. He finds the place peaceful, beautiful and intellectually stimulating. Rumor has it that he likes it so much that he is refusing to leave! His friends like to joke that he has become a tenured graduate student.

To my late grandmother.

ACKNOWLEDGEMENTS

My most sincere gratitude goes to my advisor Prof. Healey, without whose help, extreme patience and generosity my long journey towards graduation could not have been possible. Apart from his command over the subject I am always impressed by his knowledge of the history of mechanics and mathematics.

I thank Prof. Jenkins for his willingness and patience to help and for all the insightful suggestions that made this work possible.

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My whole-hearted thanks to all my friends without whom graduate school could never have been such a rich and fulfilling experience.

Last but not the least, I would like to thank the National Science Foundation for supporting my research.

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LIST OF SYMBOLS

$\mathcal{F}_n$ Normal Equilibrium Equation

$\mathcal{F}_{\mathbf{t}}$ Tangential Equilibrium Equation

$\mathcal{F}_\phi$ Concentration Equilibrium Equation

$\mathbf{v}$ Tangential Variation

v^α Component of Tangential Variation

w Normal Variation

ϕ Concentration

ψ Variation in Concentration

$\mathcal{E}$ Energy

c Bending Stiffness of the Membrane

c_g Gaussian Bending Stiffness of the Membrane

$\mathbf{x}$ Current Configuration of the Membrane

$\mathbf{X}$ Reference Configuration of the Membrane

$\mathbf{f}(\mathbf{X})$ Mapping of reference to current configuration

$\mathbf{n}(\mathbf{x})$ Normal vector parametrized by current configuration

$g_{\alpha\beta}$ Metric tensor

$b_{\alpha\beta}$ Second fundamental form

$\Gamma^{\cdot}_{\cdot\cdot}$, $\Upsilon^{\cdot}_{\cdot\cdot}$ Christoffel Symbols of generic manifolds

ϑ Polar angle in spherical coordinates

φ Azimuthal angle in spherical coordinates

dA Area form on S^2

$\boldsymbol{i}$, $\boldsymbol{j}$, $\boldsymbol{k}$ Standard cartesian basis

$a := b$ a is defined to be equal to b

$\partial_\alpha f$ The partial derivative, $\frac{\partial f}{\partial X^\alpha}$

CHAPTER 1

INTRODUCTION

Lipid membranes are an important component of all cells. Apart forming a protective covering for the various cell organelles, a lipid membrane supports a variety of essential trans-membrane proteins that play a vital role in the proper functioning of a cell.

One of the earliest attempts at modeling lipid membranes was made by Canham [9] in which he proposed the energy density of the membrane to be proportional to square of the mean curvature. Helfrich [33] extended this work by including a gaussian curvature contribution to the energy. He also laid the physical foundations for a mechanical theory of lipid bilayers. Jenkins, in [38], placed the Helfrich model within the context of modern shell theory and derived general equilibrium equations for lipid bilayer membranes. Earliest attempts to model phase transitions in lipid membranes by combining the Helfrich model for lipid membranes with the Cahn-Hilliard model can be traced to the work of Seifert [54], where he discusses the interplay between curvature and phase. A dissipative model for the dynamics of lipid membranes has been discussed by Taniguchi [60]. An alternative approach via diffuse interface modeling has been explored by Du [63].

Numerical computations for lipid bilayer membranes can be first found in the work of Jenkins [39]. Axisymmetric solutions to the Helfrich model are computed by writing the equilibrium equations as a system of first order ordinary differential equations. Nonaxisymmetric solutions in the context of two phase lipid membranes have been presented in [60]. A finite element approach to compute equilibria can be found in the work of Klug, *et. al.* [19, 48]. They employ a C^1-conforming subdivision finite element to represent membrane geometry. A parametric FEM approach to computation has been developed by Bonito *et. al.* in [6]. Elliot *et.*

al. [15, 16] use a H^1-conforming surface FEM approach for computations.

Common problems encountered in all the FEM approaches to computation in the works mentioned above are distortions of the mesh and the presence of spurious modes. Different strategies have been suggested to address these issues. Klug *et. al.* [19, 48] use a computational strategy that incorporates viscous damping effects to smoothen the mesh and spurious modes are suppressed by increasing the order of quadrature. Repeated remeshing has been suggested in [16], while Bonito, *et. al.* implement a mesh optimization routine to smoothen the mesh. Here, we present a theoretical fix using a gauge fixing procedure, discussed in detail below.

In the present work, we address certain theoretical and computational aspects of phase transition in lipid bilayer membranes. We use a popular phase field model [54, 60, 16] that combines the Helfrich model [33] for lipid bilayer membranes with the Cahn-Hilliard model [8]. In literature, there seems be a lack of concensus on the implementation of the area constraint. For these area preserving lipid membranes, some prefer a local area constraint [39, 60] while others use a global area constraint [19]. Steigman [57] partially resolved this conflict in the context of single phase lipid membranes by showing that both the formulations yield the same Euler-Lagrange equations. However, he does not address the issue of constraints. Secondly, no such resolution is offered in the context of stability. In this work, we shall extend his result by showing both formulations to be equivalent not only with respect to equilibria but also with respect to their stability. We show this in the context of the two-phase lipid membrane model.

Numerical computation of equilibria for lipid membranes is notoriously difficult. Mesh distortions, spurious modes and other numerical artifacts are often reported, as discussed above. These difficulties arise from the reparametrization symmetry of the problem, which itself is a manifestation of fluidity of the lipids.

The infinite dimensionality of this symmetry group renders the Euler-Lagrange equations underdetermined. In the special case of axisymmetry, it is possible [39] to use the locally incompressible formulation to sufficiently constrain the system and accurately compute equilibria. However, in a more general nonaxisymmetric case, such a strategy will not work; the system still has redundant degrees of freedom. Moreover, even in the axisymmetric case, if a variational approach is used to solve the Euler-Lagrange equations (perhaps, via FEM), the previously mentioned locally incompressible formulation will be difficult to implement. The (local area) point-wise constraint in this formulation will have to be enforced using a mixed formulation which is notorious for numerical instability. We shall see that this issue can be circumvented by using a global area formulation, provided the indeterminacy arising from reparametrization symmetry is appropriately (using a gauge fixing procedure, discussed below) handled.

Using physicists' terminology, reparametrization symmetry in this problem can be considered to be a *gauge symmetry*. Since gauge symmetry usually implies the existence of redundant degrees of freedom, a *gauge fixing procedure* is usually employed to break the symmetry and "fix" these extra degrees of freedom. This is done by introducing supplementary conditions to the Euler-Lagrange equations. One of our goals in this work is to propose a gauge fixing procedure for the lipid membrane problem.

With a gauge fixed formulation at hand, we systematically solve the problem computationally for equilibria and their stability. Unlike some studies [60] where computation of equilibria and their stability are combined by modeling the problem as a dissipative flow, we believe in not confusing existence and stability. Instead, we first compute equilibria by solving the discretized Galerkin formulation. Stability of these equilibria are then independently analyzed. Although we restrict this

work to axisymmetric computations, the gauge-fixing procedure that we propose is quite general. The discretized equations are studied using numerical path continuation for systematically exploring the parameter space. We also present formal arguments to show the local existence of solution branches using analytical tools from bifurcation theory.

Determining the stability of computed equilibria is a nontrivial task. Firstly, the explicit form for the second variation (hessian) is quite complex. Secondly, due to the constraints involved, the criterion for stability is more delicate than for an unconstrained problem. For an equilibrium solution to be stable, the hessian needs to be positive definite with respect to *all admissible variations* - variations that satisfy (linearized) constraints. In addition, although the solutions themselves are axisymmetric, the "full" hessian that includes both axisymmetric and nonaxisymmetric perturbations needs to be assembled. We do this efficiently through a block-diagonalized hessian by calculating its symmetry adapted basis. A constrained eigenvalue problem is then solved to determine stability.

1.1 Outline of the Thesis

We begin chapter 2 with a discussion on the phenomenology of phase transitions in lipid membranes. A well known mathematical model is subsequently introduced which combines the Cahn-Hilliard model for phase transitions with the Helfrich model for lipid membranes. Here, there are two different approaches that are traditionally taken in literature to model the area preserving property of the lipid membranes. These two approaches differ in the nature of constraints imposed - a local area constraint versus a global area constraint - each with its own set of advantages and disadvantages. However, this ambiguity of choice in a model is troubling from a theoretical point of view. In this chapter, we resolve this

ambiguity by showing the two constraints to be equivalent for lipid membranes of genus zero (in the topological sense). The Euler-Lagrange equations for the system are summarized (with derivations postponed to the appendix). We note that the Euler-Lagrange equations are underdetermined and that it stems from the in-plane fluidity of the membranes. A consequence of fluidity is the reparametrization invariance of the system. The relation between the associated symmetry group - the diffeomorphism group of S^2 - being infinite dimensional and indeterminacy inherent to the system, expressed by Nöther's second theorem, is explored briefly at the end of this chapter.

In chapter 3, a local bifurcation analysis of the system is presented. We linearize the Euler-Lagrange equations about a homogeneous spherical shape (trivial solution branch). By using formal arguments, we show the existence of local branches of solutions (up to a rigid mode and reparametrization) bifurcating from the trivial branch. However, to do this, standard tools from local bifurcation theory [46] cannot be directly applied due to the high dimensionality of the null space (of the linearization). However, this is circumvented difficulty by using group theoretic strategies [53, 23]. More specifically, this is done by looking for solution branches with a predetermined symmetry *i.e.,* invariant under a specific group action. These solutions, for the problem at hand, turn out to be symmetric spherical harmonics. In the last section of this chapter, we summarize a procedure (due to Poole [52]) that can be used to explicitly construct symmetric spherical harmonics. We apply his method to construct local symmetry-breaking branches with octahedral and icosahedral symmetry.

Chapter 4 is concerned with the question of stability. The second variation that is summarized and the details of its tedious derivation is postponed to appendix (C). The various constraints involved in the formulation makes the issue

of stability a little delicate. In particular, the choice between a local and a global area constraint seen in chapter 2 is again encountered here. Strictly speaking, since stability intricately depends on the constraints imposed, it is not obvious (*a priori*) that the two formulations must agree on stability even though they are equivalent for determining equilibria. We shall show in this chapter that even in for stability the two constraints may be treated to be equivalent as long as the membrane has a topological genus of zero. We end the chapter with a brief digression into volume control, a constraint, which turns out to be required to obtain stable equilibria. This will be taken up again in chapter 8.

In chapter 5, we return to reparametrization invariance of the energy functional that was introduced in chapter 2. As was noted in the latter, a consequence of reparametrization symmetry (due to in-plane fluidity) is the existence of grossly nonisolated solution branches - since, any arbitrary reparametrization of a solution is also a solution. In this chapter, we view this symmetry as a gauge symmetry. Ideas of gauge fixing inspired by their use in General Theory of Relativity is used to formulate a gauge fixing procedure for the lipid membrane problem. This is be done using the theory of *harmonic maps*. We show that by augmenting the governing equations of the lipid membrane with the harmonic map equation (and certain other integral constraints) it is possible to sufficiently constrain the system and break the gauge symmetry. This gauge fixing procedure, apart from an intrinsic theoretical interest, is tremendously useful for accurately computing solution branches. In particular, it avoids numerical issues such as mesh distortion and possibility of spurious modes that are frequently encountered in such problems [16, 19].

The next two chapters are concerned with computational aspects of the problem. In chapter 6, we discuss the discretization of the Euler-Lagrange equations.

We begin the chapter by recalling a few basic facts on numerical path following and then formulate the weak form using a Galerkin projection. The gauge equation that was introduced in chapter 5 is augmented to the system of equilibrium equations to derive the weak form. We end the chapter by specializing the discretized formulation to the axisymmetric case by picking appropriate spaces for shape and test functions.

Stability of the computed equilibria is the topic of interest in chapter 7. For axisymmetric solutions, stability can only be ascertained by computing the "full" hessian. The "full" hessian is contrasted with the "axisymmetric" hessian (that is used in the equilibrium computations of chapter 6) in that it carries stability information with respect to *all* allowed perturbations, as opposed to the latter which is only concerned with axisymmetric perturbations. Although, the hessian noted in chapter 4 may be routinely discretized, such a procedure will be exorbitantly expensive for computations. An efficient way to discretized and assemble the hessian is using group theoretic methods. To this end, we begin this chapter by recalling essential facts on symmetry adapted basis and block diagonalization. When the hessian is written in the symmetry adapted basis, it is block diagonalized. The individual blocks can be assembled independently and their eigenvalues can be used to assess stability. One of the main advantages of this approach is that the unnecessary zero entries of the hessian does not have to be assembled. This tremendously decreases the computational time and effort. Moreover, since the blocks may be assembled independently, parallelizing the computation is straightforward. The reminder of this chapter will be spent on computing the symmetry adapted basis of the hessian for an axisymmetric solution.

Computational results of both equilibria and their stability is summarized in chapter 8. Axisymmetric solution paths are computed using path continuation on

the discretized finite element system. The goal of the computation is to systematically look for solutions, similar to the ones observed in experiments, and ascertain their stability. A strategy developed by Healey, *et al.* [31, 30] will be used for this purpose.

CHAPTER 2

FORMULATION AND EQUILIBRIUM EQUATIONS

2.1 Introduction

In this chapter we introduce a well known model [60, 16] that is used to model phase transition in lipid membranes. It combines the Helfrich model [33] which has been successfully used [39, 19, 60] to model lipid bilayer membranes with the Cahn-Hilliard model [8] which is commonly used for phase transitions. After a brief discussion on the phenomenology of phase transition in lipid membranes, the model is introduced. Two popular versions of the formulation are commonly found in literature. These differ on the area constraints that are imposed. We discuss the two formulations by introducing their associated Helholtz energies. The associated Euler-Lagrange equations are then summarized.

We digress briefly to discuss an important symmetry of the system, namely, reparametrization invariance. This stems from the in-plane fluidity of lipid membrane. We shall see that this symmetry manifests itself as freedom to choose arbitrary coordinates to describe solutions. Thus, the system has no definitive reference configuration. Paradoxically, this freedom both simplifies and complicates the problem. On the one hand, it unifies the two formulations (that differ in the area constraints) to one equivalent formulation. On the other hand, the freedom manifests itself as an indeterminacy in the Euler-Lagrange equations which makes computations of equilibria difficult. We shall return to this latter issue in chapter 5.

We begin the next section with a brief discussion on phase transition in lipid bilayers. A more detailed discussion can be found in [12].

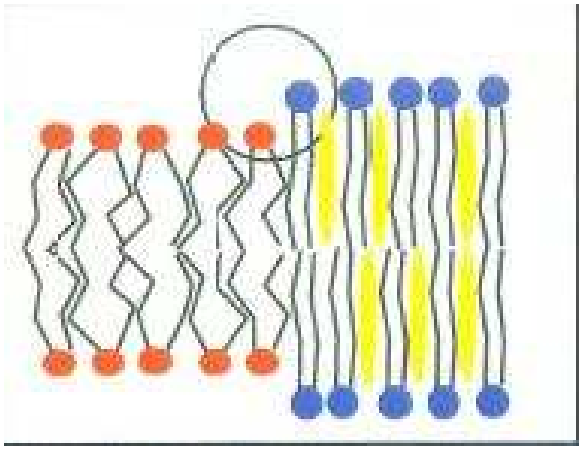


Figure 2.1: Schematic of a phase separated lipid membrane

2.2 Phenomenology of Phase Transition in Lipid Membranes

Cells of every organism are enclosed by a bilayer membrane called a cell membrane. Apart from protecting the interior of the cell, cell membranes support a variety of trans-membrane protiens that play a vital role in the proper functioning of the cell. The chemical constituents of these membranes are lipids, more commonly known as fat molecules. Structurally, lipid molecules consist of a hydrophilic head and a hydrophobic tail, schematically shown in Fig. (2.1). Under sufficient concentration of lipids, the molecules assemble themselves as bilayers membranes or even enclosed vesicles. A distinguishing feature of lipid membranes is their fluidity. At the same time, they resist bending due to hydrophic nature of the tails. Constitutively, fluidity implies that the membrane has no memory of its reference configuration in the plane of the membrane, *i.e.,* no preferred reference configuration (in-plane). Resistence to bending means that the lipid membrane keeps track of changes in normal (bending effects), similar to an elastic shell. This makes them share propertis of both a solid shell and a fluid. Liquid crystals also exhibit similar properties.

In the laboratory, lipid vesicles are synthesized by combining different kinds of lipids [5, 61] - DOPC, DPPC, Sphingomylin, to name a few. Each type of lipid are capable of exhibiting multiple structural conformations that are temperature specific. At physiologically relevant temperatures, two conformations are of particular interest, *viz.*, *Liquid-ordered*, L_o, in which the tails of the lipid molecules are all aligned and *Liquid-disordered*, L_d, in which the tails are jagged. A schematic of these two phases is shown in Fig. (2.1). These two conformations are considered to be the two liquid phases of lipids. In experiments on giant unilamellar vesicles (GUVs), [5, 61] as a control variable (pressure or temperature) is changed, phase separation is observed. Careful observation suggests that the phase transition shows all the characteristics of spinodal decomposition [62]. Figure (2.2) shows a sampling of results taken from the work of Baumgart, *et al*, [5] that were observed using confocal flouroscent microscopy. Red and Blue colors represent L_d and L_o, respectively.

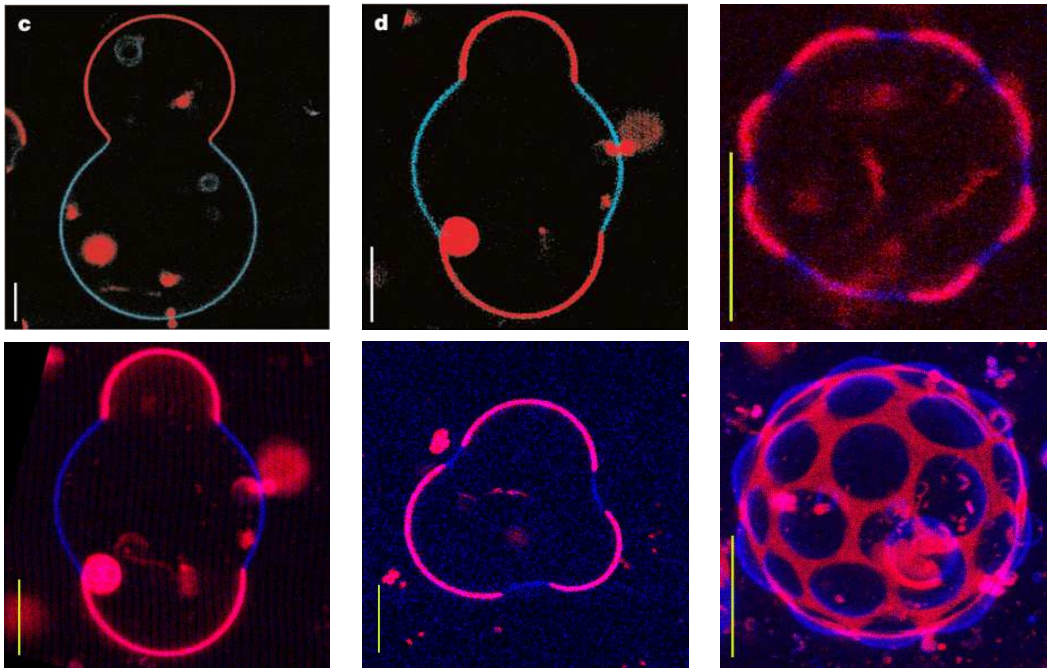


Figure 2.2: Phase transition in Giant Unilamellar Vesicles, [5].

2.3 Formulations

We assume, without loss of generality, the reference surface of the closed membrane to be a unit sphere. Let $\mathbf{X} = (X^1, X^2) \in S^2$ represent a parametrization of the unit sphere. Let $\mathbf{x} = \mathbf{f}(\mathbf{X})$, $\mathbf{f} : S^2 \to \omega \subset \mathbb{R}^3$, define an embedding of the current configuration of the membrane, ω, in $\mathbb{R}^3$.

On ω, we define a scalar field $\phi : \omega \to \mathbb{R}$ to represent the concentration variable that is responsible for phase transition. Physically, ϕ represents the difference in concentration of the two constituent lipid molecules. It is important to note that due to fluidity, it only makes sense to define ϕ on ω, the current configuration of the membrane. Explicitly, this dependence is shown by writing, $\phi = \phi(\mathbf{x})$. The concentration variable is thus invariably coupled to the shape of the surface. However, to write the Euler-Lagrange equations (discussed below) and for computations, it will be more convenient to pull the variable ϕ back to the reference surface via the mapping $\mathbf{f}$. For the sake of notational convenience, we shall abuse our notation and refer to the pull back as $\phi(\mathbf{X})$, instead of $(\phi \circ \mathbf{f})(\mathbf{X})$.

Let H and K represent the mean and gaussian curvatures of the membrane surface ω. We associate to these variables bending rigidities c and c_g, respectively [33]. The bending stiffnesses are assumed to be dependent on the molecular structure of the lipids. Accordingly, we let these stiffnesses to be , in general, functions of ϕ. Figure (2.3) shows one particular realization of this dependence.

As mentioned earlier, a successful model for bending elasticity of a single phase lipid membrane is the Helfrich model in which the internal energy density is proportional to the square of the mean curvature. Conventionally, another term proportional to the gaussian curvature is added. The proportionality constants being the bending moduli c and c_g, respectively. For closed membranes the latter term does not make any contribution to the Euler-Lagrange equations, a fact attributed

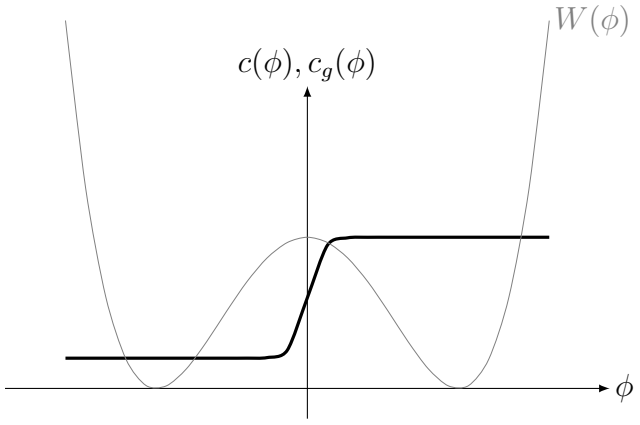


Figure 2.3: A schematic for bending stiffnesses c and c_g as a function of ϕ.

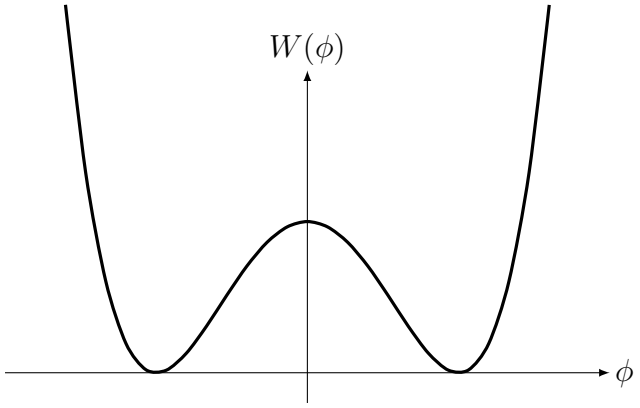


Figure 2.4: A schematic for double well potential.

to the Gauss-Bonnet theorem [39, 57]. In the model for a two phase membrane that we present below, the form for the Helfrich energy is retained, but the bending stiffnesses now depend on the concentration/ phase field. We call this energy $\mathcal{E}_H$,

$$\mathcal{E}_H = \int_\omega c(\phi)H^2 + c_g(\phi)K \; da, \tag{2.1}$$

where, da is an area measure on the current configuration, ω.

To model phase transitions, we introduce the difference in concentration of the two lipid components as the scalar field ϕ and postulate a Cahn-Hilliard type energy[8] for the field in terms of the double well potential for W (as shown in figure (2.4)),

$$\mathcal{E}_{CH} = \int_\omega W(\phi(\mathbf{x})) + \frac{\epsilon}{2}|\nabla\phi(\mathbf{x})|^2 \; da. \tag{2.2}$$

For clarity, let us write $|\nabla\phi(\mathbf{x})|^2$ explicitly in terms of reference coordinates.

$$|\nabla\phi(\mathbf{x})|^2 = g^{\alpha\beta}\partial_\alpha\phi(\mathbf{X})\partial_\beta\phi(\mathbf{X}) \; \alpha, \beta \in \{1, 2\}. \tag{2.3}$$

In the above expression, $g^{\alpha\beta}$ stands for the metric tensor of the surface ω. A concise summary of differential geometric definitions can be found in [39, 57]. Einstein summation convention is used through-out this work.

Since the phase field represents a normalized concentration difference of the components that make up the lipid membrane and the lipid components are non-reacting, we can assume that each individual component is conserved. That is, the average value of ϕ over the surface of the membrane is a fixed, let us call it μ. Thus, we have the following constraint on ϕ,

$$\int_\omega (\phi(\mathbf{x}) - \mu) \; da = 0. \tag{2.4}$$

2.3.1 Global Area Formulation

It has been observed experimentally that the area compression modulus is of the order $10^{-1}N/m$[37, 65], much higher than the bending stiffness which is of order $10^{-19}Nm$,[37]. So, to a very good approximation, the lipid membranes can be assumed to be incompressible. However, these experimental observations only imply incompressibility on average, i.e., global area preservation. Mathematically, this can be expressed by the following constraint,

$$\int_\omega da = 4\pi, \tag{2.5}$$

where 4π in the previous equation comes from our assumption that the reference sphere has a unit radius.

By combining the two energies $\mathcal{E}_H$ and $\mathcal{E}_{CH}$ with the appropriate constraints we have the following Helmholtz energy for the two phase lipid membrane system,

$$\mathcal{E}_{GA} = \int_\omega c(\phi)H^2 + c_g(\phi)K + W(\phi(\mathbf{x})) + \frac{\epsilon}{2}|\nabla\phi(\mathbf{x})|^2 \, da + \gamma\int_\omega da + \lambda\int_\omega(\phi-\mu)\, da - pV, \tag{2.6a}$$

subject to the constraints,

$$\int_\omega da = 4\pi, \tag{2.6b}$$

$$\int_\omega(\phi-\mu)\, da = 0, \tag{2.6c}$$

where γ and λ are the Lagrange multipliers enforcing the two constraints, V is the enclosed volume and p, the internal pressure.

This formulation will henceforth be referred to as GA.

2.3.2 Local Area Formulation

In the continuum mechanics community [39, 57], there is a tendency to favor local incompressiblity, where an infinitesimal area on the deformed surface and its pull

back to the reference state are considered equal. In such a formulation, we must enforce the following condition,

$$J := \frac{da}{dA} = \frac{\sqrt{g}}{\sqrt{G}} = 1. \tag{2.7}$$

The area ratio noted above is the Jacobian determinant of the mapping $\mathbf{f}$ for which we use the symbol J. The quantity G in the previous equation is the determinant of the metric tensor on the reference sphere with respect to a chosen parametrization. For example, if we choose $\mathbf{X} = (\vartheta, \varphi)$, the polar and azimuth angle, respectively, then $\sqrt{G} = \sin\vartheta$.

The Helmholtz energy for the local area formulation can be written as follows,

$$\mathcal{E}_{LA} = \int_\omega c(\phi)H^2 + c_g(\phi)K + W(\phi(\mathbf{x})) + \frac{\epsilon}{2}|\nabla\phi(\mathbf{x})|^2 \, da + \int_\omega \gamma(\mathbf{x}) \, da + \lambda \int_\omega (\phi - \mu) \, da - pV, \tag{2.8a}$$

subject to the constraints,

$$J = 1, \tag{2.8b}$$

$$\int_\omega (\phi - \mu) \, da = 0. \tag{2.8c}$$

This formulation will henceforth be referred to as LA. Note the explicit dependence of γ on $\mathbf{x}$ in this formulation. This is required for enforcing the pointwise constraint $J = 1$.

In general, the two constraints are not equivalent. Steigman [57] has shown that in the case of the Helfrich model, the governing equations for the constraints are identical. He uses this to conclude that the models are equivalent. However, the argument to show this equivalence is a little more delicate. Having identical governing PDE does not guarantee the equivalence of models. Equivalence of constraint equations should also be established. Nevertheless the conclusion is

indeed correct. In what follows, We shall show that for membranes of genus zero, equivalence of area constraints is indeed true.

Until we establish this equivalence we shall, keeping in the spirit of continuum mechanics, assume local incompressibility of area.

2.4 Euler-Lagrange Equations

To derive the Euler-Lagrange equations we must take the variation of the energy with respect the unknowns $\mathbf{f}$ and ϕ. It is well known in literature [57], [39] that the most convenient way to write the Euler-Lagrange equations is by taking variations of the deformation field $\mathbf{f}$ in the normal and tangential directions,

$$\mathbf{x} = \mathbf{f} \rightarrow \mathbf{f} + \alpha\delta\mathbf{f} = \mathbf{x} + \alpha\Big(\mathbf{v}(\mathbf{x}) + w(\mathbf{x})\mathbf{n}(\mathbf{x})\Big), \tag{2.9}$$

where $\mathbf{v}$ is tangential variation relative to ω, w is the component of the normal variation (with respect to ω) and $\mathbf{n}(\mathbf{x})$ is the normal at the point $\mathbf{x}$ on ω.

For taking the correct variation in concentration, it is crucial to note that concentration, $\phi(\mathbf{x})$, is a function of the current configuration, $\mathbf{x} = \mathbf{f}(\mathbf{X})$. Thus, the variation in concetration has two contributions - 1) due to variation of the field ϕ 2) due to variation of the current configuration itself. If ψ represents the variation in concentration, then for sufficiently small α,

$$\phi(\mathbf{x}) \mapsto \phi(\mathbf{x}) + \alpha\Big(\delta\phi(\mathbf{x})\Big). \tag{2.10}$$

But since $\mathbf{x} = \mathbf{f}(\mathbf{X}) \mapsto \mathbf{f}(\mathbf{X}) + \alpha(\mathbf{v} + w\mathbf{n})$

$$\phi(\mathbf{x}) = \phi(\mathbf{f}(\mathbf{X})) \mapsto \phi(\mathbf{f}(\mathbf{X}) + \alpha(\mathbf{v} + w\mathbf{n})) + \alpha[\psi(\mathbf{f}(\mathbf{X}))],$$

that is,

$$\phi(\mathbf{x}) \mapsto \phi(\mathbf{x}) + \alpha[\psi(\mathbf{x}) + \nabla\phi(\mathbf{x}) \cdot \mathbf{v}]. \tag{2.11}$$

Therefore, the variation in concentration, ψ, can be written as

$$\delta\phi = \psi(\mathbf{x}) + \nabla\phi \cdot \mathbf{v}, \tag{2.12}$$

where the term $\nabla\phi \cdot \mathbf{v}$ represents the convected contribution to the variation due to the variation in the surface itself.

To derive the Euler-Lagrange equations, we set the first variation of the energy (2.8a) with respect to the variables $\mathbf{f}$ and ϕ to zero,

$$\frac{d}{d\alpha}\mathcal{E}(\mathbf{f} + \alpha\delta\mathbf{f}, \phi + \alpha\delta\phi)\Big|_{\alpha=0} = 0. \tag{2.13}$$

Details of the calculation can be found in the Appendix (B). We have the following Euler-Lagrange equations,

$$\tilde{\Delta}c_g(\phi) + \Delta(cH) + 2cH(H^2 - K) + \epsilon\mathbf{b}[\nabla\phi, \nabla\phi] - 2\tilde{\gamma}H - p = 0, \tag{2.14a}$$

$$\epsilon\nabla \cdot (\nabla\phi \otimes \nabla\phi) - (\epsilon\Delta\phi - W' - \lambda)\nabla\phi - \nabla\tilde{\gamma} = \mathbf{0}, \tag{2.14b}$$

$$-\epsilon\Delta\phi + W'(\phi) + c'H^2 + c_g'K + \lambda = 0, \tag{2.14c}$$

where, $\mathbf{b}$ is the curvature tensor, $\tilde{b}^{\alpha\beta}$ is the cofactor of the curvature tensor, $\tilde{\Delta}\cdot = \tilde{b}^{\alpha\beta}\nabla_\alpha\nabla_\beta$, and

$$\tilde{\gamma} = \frac{\epsilon}{2}|\nabla\phi|^2 + W + \lambda(\phi - \mu) + \gamma. \tag{2.14d}$$

Remark 1. *Note that in the case of the GA formulation, since γ is a constant, $\nabla\gamma \equiv 0$.*

2.5 Reparametrization Symmetry

Let us note the Helmholtz energy of the GA formulation, (2.6a) and its associated constraints (2.6b),(2.6c) are invariant under coordinate reparametrization. That is, for any diffeomorphism $\chi : S^2 \to S^2$,

$$\mathcal{E}_{GA}(\mathbf{f}(\mathbf{X}), \phi(\mathbf{X})) = \mathcal{E}_{GA}(\mathbf{f} \circ \chi(\mathbf{X}), \phi \circ \chi(\mathbf{X})).$$

This means that if $(\mathbf{f}^*(\mathbf{X}), \phi^*(\mathbf{X}))$ is any solution to the Euler Lagrange equations (2.14) and the associated GA constraints (2.6a)(2.6b), then $(\mathbf{f}^* \circ \chi(\mathbf{X}), \phi^* \circ \chi(\mathbf{X}))$ is also a solution to the system, for any diffeomorphism $\chi : S^2 \to S^2$.

Another way to see this result is to recognize that the differential equations (2.14) and the associated global integral constraints do not explicitly depend on any coordinate system. So, there is freedom to choose any coordinate system on the sphere. As a consequence, solutions to the GA formulation always exists as an infinite dimensional equivalence class, where two solutions are considered equivalent if there is a diffeomorphism relating them. We call this freedom to choose any coordinates to describe a solution as *gauge freedom*. We shall return to this in chapter 5.

It is important to note that the local area constraint is not invariant under arbitrary reparametrizations of the sphere. It is, however, invariant under unimodular diffeomorphisms of the sphere.

2.6 Equivalence of Formulations

In this section, we show that for surfaces of genus zero, the LA formulation is equivalent to the GA formulation. Let us first note the following identity,

Proposition 1. *For any scalar function $f : \omega \to \mathbb{R}$, we have the following identity,*

$$\nabla \cdot (\nabla f \otimes \nabla f) = \frac{1}{2}\nabla |\nabla f|^2 + \nabla f \Delta f. \tag{2.15}$$

Proof.

$$l.h.s = (f_\alpha f^\beta)_{;\beta} = f_\alpha f^\beta_{;\beta} + f_{\alpha;\beta} f^\beta = f_\alpha f^\beta_{;\beta} + f_{\beta;\alpha} f^\beta. \tag{2.16}$$

The last equality follows from the symmetry of the Christoffel symbols. So,

$$l.h.s = f_\alpha f^\beta_{;\beta} + \frac{1}{2}(f_\beta f^\beta)_{;\alpha} = r.h.s. \tag{2.17}$$

□

Using the previous proposition in tangential equation 2.14b,

$$\epsilon \nabla \cdot (\nabla \phi \otimes \nabla \phi) - (\epsilon \Delta \phi - W' - \lambda)\nabla \phi - \left[\nabla \gamma + \frac{\epsilon}{2}\nabla |\nabla \phi|^2 + (W' + \lambda)\nabla \phi\right] = \mathbf{0}, \tag{2.18}$$

we have,

$$\nabla \gamma = 0. \tag{2.19}$$

That is

$$\gamma = C, \text{ a constant.} \tag{2.20}$$

Recall that in the GA formulation, the Lagrange multiplier γ is a constant. Thus, the equilibrium equations for the GA and the LA formulations are identical - with γ being a constant in both cases. This alone does not imply the equivalence of the two formulations, since the constraints (more specifically, the area constraints) imposed on the two formulations are not the same. However, it is true that solution set of the local area formulation is contained in the global area formulation. To see

this we note that the global area constraint may be recovered simply by integrating the local area constraint.

We shall now proceed to demostrate that in the case of surfaces with genus zero, the converse is indeed true.

Let us first recall that the every solution to the global formulation comes in an equivalence class. For the converse argument, it is sufficient to find a representative of this solution in this equivalence class that satisfies the local area constraint. To be precise, we must show that any solution $(\mathbf{f}(\mathbf{X}), \phi(\mathbf{X}))$ of the GA formulation may be mapped by a coordinate change to a solution of the LA formulation. We shall show this by explicitly constructing such a change of coordinates.

Without loss of generality we set $\mathbf{X} = (\vartheta, \varphi)$, the canonical spherical coordinates. Consider the following mapping

$$(\tilde{\vartheta}, \tilde{\varphi}) : S^2 \to S^2, \tag{2.21}$$

where,

$$\tilde{\vartheta}(\vartheta) = \arccos\left[\frac{1}{2\pi}\left(2\pi - \int_0^{\vartheta}\int_0^{2\pi} \sqrt{g}(\sigma,\tau)\, d\tau d\sigma\right)\right], \tag{2.22}$$

$$\tilde{\varphi}(\vartheta,\phi) = 2\pi \frac{\int_0^{\varphi} \sqrt{g}(\vartheta,\tau)\, d\tau}{\int_0^{2\pi} \sqrt{g}(\vartheta,\tau)\, d\tau}. \tag{2.23}$$

It is well-known consequence of Riemann-Roch theorem, [41] (cf. Chapter (5)), that genus zero surfaces are conformally equivalent to a sphere. That is, there exists a coordinate system $(\vartheta, \varphi) \in S^2$ such that the metric tensor of the surface has the following form,

$$ds^2 = \lambda^2(\vartheta,\varphi)\left(d\vartheta^2 + \sin^2\vartheta d\varphi^2\right),$$

where $\lambda^2(\vartheta,\varphi)$ is positive.

Therefore, in such a coordinate system $\sqrt{g} = \lambda^2 \sin\vartheta$ is a positive function on $(0,\pi)\times[0,2\pi]$. As a result, the integrals in the equations (2.22),(2.23) are monotone functions of θ and ϕ, respectively. This makes $\tilde{\vartheta}(\vartheta)$ and $\tilde{\varphi}(\vartheta,\varphi)$ invertible functions of ϑ and φ, respectively.

The following conditions follow naturally from the definitions (2.22), (2.23),

$$\tilde{\vartheta}(0) = \tilde{\varphi}(\vartheta, 0) = 0, \text{ for every } \vartheta \in [0,\pi]. \tag{2.24}$$

Noting the global area constraint

$$\int_0^{\pi}\int_0^{2\pi} \sqrt{g}(\sigma,\tau)\, d\tau d\sigma = \int_{\omega} da = 4\pi, \tag{2.25}$$

we can also conclude the following conditions

$$\tilde{\vartheta}(\pi) = \pi, \ \tilde{\varphi}(\vartheta, 2\pi) = 2\pi, \text{ for all } \vartheta \in [0,2\pi]. \tag{2.26}$$

We have thus demonstrated that

$$(\tilde{\vartheta},\tilde{\varphi}) : S^2 \to S^2 \tag{2.27}$$

is a diffeomorphism of a unit sphere and therefore a well defined change of coordinates.

It is a straightforward calculation to see that

$$\sqrt{g}(\vartheta,\varphi) = \sin(\tilde{\vartheta}(\vartheta)) \det\left(\frac{\partial(\tilde{\vartheta},\tilde{\varphi})}{\partial(\vartheta,\varphi)}\right). \tag{2.28}$$

That is to say, we have produced a coordinate system *viz.,* $(\tilde{\vartheta},\tilde{\varphi})$, in which $\sqrt{g}$ takes the form of $\sin\tilde{\vartheta}$. In such a coordinate system we have $J = 1$. More precisely,

$$\tilde{J}(\tilde{\vartheta},\tilde{\varphi}) = 1.$$

We have just proved the following theorem,

Theorem 1. *Any solution of the GA formulation can be mapped through a coordinate change to a solution of the LA formulation and conversely, any solution of the LA formulation is a solution of the GA formulation. That is,*

$$LA \iff GA.$$

2.7 Nöther's Second Theorem and Reparametrization Invariance

In the previous section, we saw that for the GA formulation, the tangential equation vanishes identically and therefore makes the formulation underdetermined. It will now be shown that this redundancy in the Euler-Lagrange equations is due to the reparametrization symmetry of the GA formulation.

For any $\chi \in \text{Diff}(S^2, S^2)$,

$$\mathcal{E}_{GA}(\mathbf{f}(\mathbf{X}), \phi \circ \mathbf{f}(\mathbf{X})) = \mathcal{E}_{GA}(\mathbf{f} \circ \chi(\mathbf{X}), (\phi \circ \mathbf{f}) \circ \chi(\mathbf{X})). \tag{2.29}$$

For sufficiently small ξ, $\mathbf{X} \mapsto \mathbf{X} + \xi\mathbf{V}$ defines a diffeomorphism of S^2, where $\mathbf{V}$ is a smooth tangent field on S^2. Using this as the diffeomorphism in Eq. (2.29), we have, for sufficiently small ξ,

$$\begin{aligned}\mathcal{E}_{GA}(\mathbf{f}, \phi) &= \mathcal{E}_{GA}(\mathbf{f}(\mathbf{X} + \xi\mathbf{V}), \phi \circ \mathbf{f}(\mathbf{X} + \xi\mathbf{V})) \\ &= \mathcal{E}_{GA}(\mathbf{f} + \xi\nabla\mathbf{f}\,\mathbf{V}, \phi + \xi\nabla\phi \cdot \nabla\mathbf{f}\,\mathbf{V}).\end{aligned}$$

Since $\mathbf{V}$ is a tangent field on S^2, $\mathbf{v} := \nabla\mathbf{f}\,\mathbf{V}$ defines a tangent field on ω. So, for sufficiently small ξ, we have,

$$\mathcal{E}_{GA}(\mathbf{f}, \phi) = \mathcal{E}_{GA}(\mathbf{f} + \xi\mathbf{v}, \phi + \xi\nabla\phi \cdot \mathbf{v}).$$

The previous equation leads to the following condition,

$$\frac{d}{d\xi}\mathcal{E}_{GA}(\mathbf{f} + \xi\mathbf{v}, \phi + \xi\nabla\phi \cdot \mathbf{v})\Big|_{\xi=0} \equiv 0.$$

Note that the left side of the previous equation is the tangential variation of the energy. In other words, we have demonstrated that a consequence of reparametrization symmetry is the vanishing of the tangential Euler-Lagrange equations (of the GA formulation).

This relation between redundancy in the Euler-Lagrange equations and the presence of an infinite dimensional Lie group of symmetry is called Nöther's second theorem [7].

2.8 Summary: Equilibrium Equations

In this section we summarize the equilibrium equations that will referred to in the remainder of this work.

As a result of the equivalence of the LA and the GA formulations that was demonstrated above, we have the liberty of choosing any one formulation. We choose to work with the latter particularly fot the convenience it offers towards computations. The integral constraints in this formulation make it very suitable for finite element implementation. We do wish to emphasize a draw back of the GA formulation. It is inherently underdetermined with two partial differential equations and four unknowns (three for $\mathbf{f}$ and one for ϕ). We address a method to deal with this indeterminacy in chapter 5.

We now summarize the differential equations for the system,

$$\tilde{\Delta} c_g(\phi) + \Delta(cH) + 2cH(H^2 - K) + \epsilon \mathbf{b}[\nabla\phi, \nabla\phi] - 2\tilde{\gamma} H - p = 0, \tag{2.30a}$$

$$-\epsilon\Delta\phi + W'(\phi) + c' H^2 + c'_g K + \lambda = 0, \tag{2.30b}$$

which satisfy the following constraints,

$$\int_\omega da = 4\pi, \tag{2.30c}$$

$$\int_\omega (\phi - \mu)\, da = 0, \tag{2.30d}$$

where,

$$\tilde{\gamma} = \frac{\epsilon}{2}|\nabla\phi|^2 + W + \lambda(\phi - \mu) + \gamma. \tag{2.30e}$$

We shall abstractly refer to the previous system of equations (2.30) as

$$\mathcal{F}(\mathbf{f}, \phi) = 0. \tag{2.31}$$

CHAPTER 3

BIFURCATION ANALYSIS

3.1 Introduction

In this chapter we use formal arguments to do a local bifurcation analysis of the problem. The equilibrium equations are linearized about a spherical homogeneous state, considered to be the trivial solution. The rich $O(3)$ symmetry manifests as a high dimensional null space for the linearized problem. A straightforward application of the techniques of bifurcation theory to a degenerate problem such as this is not an easy task. Fortunately, symmetry - the very cause of this degeneracy - can be used to our advantage to simplify the analysis using group theoretic strategies that have been developed by Sattinger [53], Golubitsky, *et al* [23] and successfully applied to bifurcation problems of nonlinear elasticity by Healey, [26] and others.

The essential idea in such group theoretic methods is to choose, *a priori*, a symmetry subgroup of $O(3)$ so that we have a one-dimensional fixed point space of solutions. Classification of such subgroups already exists in literature [23]. Furthermore, it can be shown that a consequence of symmetry (via equivariance) is that the fixed point space of the subgroup is an invariant subspace for the nonlinear PDE. When restricted to such a fixed point space, the tools of bifurcation theory can be readily applied. We shall show that the Crandall-Rabinowitz crossing condition [11] is readily satisfied and we shall thus establish the existence of local symmetry-breaking branches in each of the fixed point spaces.

Although one dimensional fixed point spaces under various symmetry subgroups of $O(3)$ have been tabulated [23], discussions on explicitly characterizing the basis vectors for such spaces (which give the local bifurcation directions for

the problem) has been limited in literature. In the last section of this chapter we present an algorithm for constructing these bifurcation directions. The material in this section is based on the classic paper of Poole [52] on the construction of spherical harmonics with symmetry. We choose the octahedral and icosahedral groups as two sample examples to illustrate this method.

3.2 Linearization and Local Bifurcation Analysis

Let us first note that a spherical shape ($H = -1$) with a homogeneous concentration distribution $\phi \equiv \mu$ is a solution to the system (2.30), provided $p = 2(W(\mu)+\gamma)$. This solution branch will be considered to be the *trivial branch*. We linearize the Euler-Lagrange system about this trivial branch. For convenience, we restrict ourselves to the constant bending stiffness case where $c(\phi)$ and $c_g(\phi)$ are independent of ϕ. Let $\hat{h}$ and $\hat{\phi}$ represent the perturbations of the mean curvature H and the concentration field ϕ, respectively, while $\hat{\gamma}$ and $\hat{\lambda}$ are the linearizations of the Lagrange multipliers γ and λ, respectively. Straightforward linearization of the equilibrium equations (2.30) yields the following system,

$$c\Delta^o\hat{h} - p\hat{h} = -2\hat{\gamma}, \tag{3.1a}$$

$$-\epsilon\Delta^o\hat{\phi} + W''(\mu)\hat{\phi} = \hat{\lambda}, \tag{3.1b}$$

$$\int_{S^2} \hat{\phi}\, dA = 0, \tag{3.1c}$$

$$\int_{S^2} \hat{w}\, dA = 0, \tag{3.1d}$$

where $\hat{w}$ is the perturbation of the displacement field in the direction normal to S^2 and Δ^o is the Laplace-Beltrami on S^2. The perturbation $\hat{w}$ is related to $\hat{h}$ through the following compatibility equation,

$$\Delta^o\hat{w} + 2\hat{w} = \hat{h}. \tag{3.2}$$

It is clear from the linearized system above that (up to the first order) there is no coupling between the shape and the concentration field, since equations (3.1a) and (3.1b) are independent of one another. This, however, does not imply that the lack of shape-phase interaction in the nonlinear system (2.30). The decoupling only holds close to the trivial solution (and in the case of constant bending stiffness). We shall see through our computational results in chapter (8) that for solutions sufficiently far away from the trivial branch, there is indeed a shape-phase coupling.

It is interesting to note that perturbations of displacement in the tangential direction (to S^2), $\hat{\mathbf{v}}$, do not appear in the linearization. Therefore, any arbitrary tangent field $\hat{\mathbf{v}}$ of S^2 is a null vector of the linearization. In this case, $\hat{\mathbf{v}}$ actually represents an arbitrary infinitesimal reparametrization of the sphere. We also note in passing that the term involving the Gaussian bending stiffness c_g falls out by Gauss-Bonnet.

Integrating the compatibility equation (3.2), and using the divergence theorem, we have

$$\int_{S^2} \hat{h}\, dA = 2 \int_{S^2} \hat{w}\, dA = 0, \tag{3.3}$$

where the last equality follows by using the linearized constraint equation (3.1d).

A similar argument applied to (3.1a) and (3.1b) in conjunction with the observation (3.3) is used conclude that $\hat{\gamma}$ and $\hat{\lambda}$ are both zeroes. Equations (3.1a) and (3.1b) can now be rewritten as follows,

$$c\Delta^o\hat{h} - p\hat{h} = 0, \tag{3.4a}$$

$$-\epsilon\Delta^o\hat{\phi} + W''(\mu)\hat{\phi} = 0. \tag{3.4b}$$

Nontrivial solutions to the first equation, (3.4a), can exist only for negative values of p which represent external excess pressure. These modes correspond to the shell buckling modes. Since we are primarily interested in isolating the effect of non-uniform concentration (phase) distribution on the surface of the membrane, we

disregard buckling instabilities and assume that the vesicle to be pressurized from the inside, *i.e.,* $p > 0$. Thus, the only allowed solutions to (3.4a) are the trivial solutions,

$$\hat{h} = 0.$$

As a consequence, nontrivial solutions to the system (3.4) are, only possible by choosing μ to lie in the spinodal region of the double well potential shown in figure (2.3), where $W''(\mu)$ is negative. The eigenvalue problem, (3.4b), admits nontrivial solutions if only if,

$$\frac{W''(\mu)}{\epsilon} = -l(l+1), \text{ where } l \in \{1, 2, \cdots\}. \tag{3.5}$$

In spherical coordinates (ϑ, φ), these solutions can be expressed in terms of spherical harmonics (cf. section. 3.3),

$$\hat{\phi}_l = Y_{lm}(\vartheta, \varphi), \tag{3.6}$$

where $l \in \{1, 2, 3, \cdots\}$, $m \in \{-l, -l+1, \cdots, l-1, l\}$.

It is clear from the preceding discussion that null space of the linearization is degenerate with a dimension of $2l + 1$ for each l. The cause of this degeneracy is the rich $O(3)$ symmetry of the problem. Applying the standard results of local bifurcation analysis for such a degenerate case is not a straightforward. It was first recognized by Sattinger [53] that the inherent symmetry could be used to "mod-out" this degeneracy so that tools from local bifurcation theory can be routinely applied. This approach has been successfully used in the context on problems of nonlinear elasticity in [28], [31].

Mathematically, the notion of symmetry of a system is expressed via the equivariance of its equilibrium equations under a certain group action - $O(3)$ - for the system under consideration. In the following section, we demonstrate the equivariance of the equilibrium equations (2.31) under $O(3)$-action.

3.2.1 Equivariance under $O(3)$

We first define representations of $O(3)$ on $\mathbf{f}$ and ϕ respectively,

$$\sigma\mathbf{f}(\mathbf{X}) := \boldsymbol{\sigma}\mathbf{f}(\boldsymbol{\sigma}^{-1}\mathbf{X}),$$

$$\sigma\phi(\mathbf{x}) := \phi(\sigma^{-1}\mathbf{x}) = \phi \circ \mathbf{f}(\boldsymbol{\sigma}^{-1}\mathbf{X}),$$

where $\boldsymbol{\sigma}$ is the standard representation of $O(3)$ on S^2. It can be shown that [27] the above definitions induce the following representation on H and K

$$\sigma H(\mathbf{x}) = H(\sigma^{-1}\mathbf{x}),\ \sigma K(\mathbf{x}) = K(\sigma^{-1}\mathbf{x}).$$

Further, we note the following representations,

$$\sigma\Delta(c(\phi)H(\mathbf{x})) = \Delta(c(\sigma\phi)H(\sigma^{-1}\mathbf{x})) = \Delta(\sigma(cH)),$$

$$\sigma\tilde{\Delta}c_g(\phi) = \tilde{\Delta}c_g\Big(\phi(\sigma^{-1}\mathbf{x})\Big) = \tilde{\Delta}c_g(\sigma\phi),$$
$$\sigma|\nabla\phi|^2 = \Big|\nabla\Big(\phi(\sigma^{-1}\mathbf{x})\Big)\Big|^2 = |\nabla(\sigma\phi)|^2.$$

A term-by-term application of the previous results to the equilibrium equations (2.30), gives us the desired equivariance. This fact can be abstractly summarized as follows,

$$\sigma\mathcal{F}(\mathbf{f},\phi) = \mathcal{F}(\sigma\mathbf{f},\sigma\phi).$$

3.2.2 Local Existence of Branches

Establishing local existence of branches by using standard techniques of bifurcation theory is not straightforward due to the high dimensionality for null space of linearization. However, in conjunction with equivariance established above, bifurcation theory can be used to establish local existence. This idea of using symmetry to establish local existence was developed by [53], [23]. The essential idea of this

method is to reduce the problem to a one-dimensional bifurcation problem by choosing specific symmetry types for solutions by restricting the problem to a one dimensional fixed point space of solutions. On this space, the results from 1-d bifurcation theory can be routinely applied.

Let us first note the following useful notation. Let Y, formally, represent an appropriate solution space. We have,

$$\mathcal{F} : Y \to Y.$$

The notion of symmetry of solutions can be formalized by the following definition,

Definition 1 (Fixed Point Space)**.** *For any subgroup $\Sigma \subset O(3)$, we define the* fixed point space*, Y_Σ as the set,*

$$Y_\Sigma := \{\mathbf{y} \in Y : \sigma\mathbf{y} = \mathbf{y}, \sigma \in \Sigma\}.$$

An important observation for establishing existence is the following straightforward theorem [23] which follows from the equivariance of the equilibrium equations.

Theorem 2. *The fixed point space Y_Σ is invariant under the equivariant mapping $\mathcal{F}$. That is,*

$$\mathcal{F}|_{Y_\Sigma} : Y_\Sigma \to Y_\Sigma. \tag{3.7}$$

It is remarkable that equivariance forces a nonlinear mapping $\mathcal{F}$ have a linear invariant subspace.

If the fixed point space Y_Σ is one dimensional, the system $\mathcal{F}|_{Y_\Sigma}(\mathbf{f}, \phi)$ is a one dimensional problem and techniques of one dimensional bifurcation theory can be readily applied. The fixed point space Y_Σ, can be chosen to be one dimensional by appropriately choosing Σ. The classification theorem due to Golubitsky, *et al*

[23], is tremendously useful to find all such subgroups Σ and consequently, all the possible one dimensional fixed point spaces of the subgroups of $O(3)$.

Let us abstractly represent the linearized equations (3.4), about the trivial solution as follows

$$D_{\mathbf{y}}\mathcal{F}(\mathbf{e}_r,\mu;\epsilon)\Big[\hat{w}\mathbf{n}+\hat{\mathbf{v}},\hat{\phi}\Big] := \begin{cases} c\Delta^o\hat{h}-p\hat{h}=0, \\ -\epsilon\Delta^o\hat{\phi}+W''(\mu)\hat{\phi}=0, \end{cases}$$

where $D_{\mathbf{y}}\mathcal{F}$ is the Fréchet derivative of $\mathcal{F}$ with respect to $(\mathbf{f},\phi)$. For the sake of clarity, the dependence of the derivative on parameters that are not relevant to the analysis below has been suppressed.

We strategically choose the subgroup Σ so that the results of bifurcation theory [46] can be applied to the restricted problem (3.7). For this we choose $\Sigma \subset O(3)$ such that,

$$\dim\mathcal{N}\Big(D_{\mathbf{y}}\mathcal{F}(\mathbf{e}_r,\mu;\epsilon_l)\Big|_{Y_\Sigma}\Big)=1, \tag{3.8}$$

where $\mathcal{N}$ represents the null space and ϵ_l is the solution to the characteristic equation (3.5) for a particular choice of l for which nontrivial solutions to the linearization exist.

The sufficient condition for bifurcation, namely the Crandall-Rabinowitz crossing condition [11] can be readily checked. Indeed,

$$\langle \mathbf{y}_l, D^2_{\mathbf{y}\epsilon}\mathcal{F}^o[\mathbf{y}_l]\rangle = l(l+1)\neq 0, \text{ for any } \mathbf{y}_l\in\mathcal{N}\Big(D_{\mathbf{y}}\mathcal{F}^o(\epsilon_l)\Big|_{Y_\Sigma}\Big), \tag{3.9}$$

Therefore, up to reparametrization and rigid modes, there exists, in the neighborhood of the trivial solution, a symmetry-breaking solution path to the equation $\mathcal{F}|_{Y_\Sigma}=0$ in Y_Σ (that is, with Σ as its symmetry). Moreover, these solutions have the following form,

$$\mathbf{f}(\epsilon)=\mathbf{e}_r+o(\epsilon), \tag{3.10a}$$

$$\phi(\epsilon)=\mu+\epsilon Y_l^\Sigma+o(\epsilon), \tag{3.10b}$$

for ϵ sufficiently close to ϵ_l. Here Y_l^Σ is a spherical harmonic of order l that is $\Sigma-$symmetric.

The subgroups Σ, of $O(3)$ with a one dimensional fixed point spaces has been classified, the details of which can be found in [23]. For instance, for $l = 4$ the octahedral subgroup admits a one dimensional fixed point space, where as for $l = 6$ the icosahedral subgroup has a one dimensional fixed point space. Both these examples are discussed below.

3.3 Spherical Harmonics with Polyhedral Symmetry

In this section we outline a procedure to explicitly compute the fixed point spaces of a symmetry subgroup $\Sigma \subset O(3)$. We summarize a well known procedure [52] for generating spherical harmonics having symmetries of a platonic solid. No originality is claimed in this section.

3.3.1 Spherical Harmonics

In this section we review a few facts about spherical harmonics. Consider the problem,

$$\Delta y = 0, \text{ on } \mathbb{R}^3, \tag{3.11}$$

where $y : \mathbb{R}^3 \to \mathbb{R}$.

Using separation of variables in terms of the canonical spherical coordinates (r, ϑ, φ) we write $y = R(r)Y(\vartheta, \varphi)$. The previous PDE can then be rewritten as follows

$$\Delta^o Y + \lambda Y = 0, \tag{3.12a}$$

$$\frac{d}{dr}(r^2 \frac{dR}{dr}) - \lambda R = 0, \tag{3.12b}$$

where Δ^o is the Laplace-Beltrami on the S^2 and λ is a constant.

It can be shown that [35] (3.12a) admits non-trivial solution if and only if $\lambda = l(l+1)$ where $l \in \{0, 1, 2, \cdots\}$. *Spherical harmonics*, Y_l, are defined to be the non-trivial solutions to this equation. In other words, they are the eigen functions of the Laplace-Beltrami operator on S^2, Δ^o. That is,

$$-\Delta^o Y_l = l(l+1)Y_l. \tag{3.13}$$

For every non-negative integer choice of l the above equation has $2l+1$ linearly independent solutions [35], conventionally labelled as Y_{lm}, where $m \in \{-l, -l+1, \cdots, l-1, l\}$. These solutions can be explicitly expressed in terms of the *associated Legendre polynomials*, P_{lm} as follows

$$Y_{lm}(\vartheta, \varphi) = \begin{cases} P_{lm}(\cos\vartheta)\cos m\varphi, \text{ if } m > 0, \\ P_{l|m|}(\cos\vartheta)\sin|m|\varphi, \text{ if } m < 0. \end{cases} \tag{3.14}$$

Combining the solutions of the system (3.12), the solutions to the Laplace equation on $\mathbb{R}^3$, (3.11), can be written as,

$$y_l = r^l Y_{lm}(\vartheta, \varphi), \tag{3.15}$$

where $l \in \{0, 1, 2, \cdots\}$ and $m \in \{-l, -l+1, \cdots, l-1, l\}$.

It will be important in the following development to note the following fact

$$Y_{lm} = y_l|_{r=1}. \tag{3.16}$$

That is, spherical harmonics are restrictions of harmonic functions on $\mathbb{R}^3$ to a unit sphere.

We now proceed to demonstrate Poole's method to construct the Σ-symmetric spherical harmonics. It is based on Maxwell's method of multipoles of writing a spherical harmonic of order n in terms of an n^{th} directional derivatives of $1/r$, where $r = \sqrt{x^2+y^2+z^2}$ [50]. Sylvester [59] showed that Maxwell's derivative expansion was unique (up to reordering of derivatives).

In the following section, we provide the proof for Maxwell's method of multipoles. The proof for the uniqueness result of Sylvester is more involved and we direct the reader to his paper [59].

3.3.2 Maxwell and Sylvester Theorems

We introduce the following definition $r := |\mathbf{r}|$, for notational convenience.

We will need the following lemmas,

Lemma 1.

$$\frac{d}{d\alpha}|\mathbf{r}+\alpha\boldsymbol{\eta}||_{\alpha=0} = \frac{\mathbf{r}\cdot\boldsymbol{\eta}}{|\mathbf{r}|}. \tag{3.17}$$

Proof.

$$\begin{aligned}\frac{d}{d\alpha}|\mathbf{r}+\alpha\boldsymbol{\eta}||_{\alpha=0} &= \frac{d}{d\alpha}\sqrt{|\mathbf{r}+\alpha\boldsymbol{\eta}|^2}|_{\alpha=0}\\ &= \frac{1}{2|\mathbf{r}|}\frac{d}{d\alpha}\langle\mathbf{r}+\alpha\boldsymbol{\eta},\mathbf{r}+\alpha\boldsymbol{\eta}\rangle|_{\alpha=0}\\ &= \frac{\mathbf{r}\cdot\boldsymbol{\eta}}{|\mathbf{r}|}.\end{aligned}$$

□

Lemma 2.

$$\nabla\left(\frac{1}{r}\right) = -\frac{\mathbf{r}}{r^3}. \tag{3.18}$$

Proof.

$$\nabla\left(\frac{1}{r}\right)\cdot\boldsymbol{\eta} = \frac{d}{d\alpha}\Big[\frac{1}{|\mathbf{r}+\alpha\boldsymbol{\eta}|}\Big]_{\alpha=0} = -\frac{1}{|\mathbf{r}|^2}\frac{d}{d\alpha}|\mathbf{r}+\alpha\boldsymbol{\eta}|_{\alpha=0}.$$

Now using Lemma (1), we conclude,

$$\nabla\left(\frac{1}{r}\right)\cdot\boldsymbol{\eta} = -\frac{\mathbf{r}}{r^3}\cdot\boldsymbol{\eta}.$$

□

The following corollary follows from the previous lemma.

Corollary 1.

$$\nabla\left(\frac{1}{r^{2n+1}}\right) = -\frac{(2n+1)\mathbf{r}}{r^{2n+3}},\ \textit{for any } n. \tag{3.19}$$

Lemma 3.

$$\Delta\left(\frac{1}{r^{2n+1}}\right) = \frac{2n(2n+1)}{r^{2n+3}}. \tag{3.20}$$

Proof.

$$\Delta\left(\frac{1}{r^{2n+1}}\right) = \nabla\cdot\nabla\left(\frac{1}{r^{2n+1}}\right).$$

Now using Cor. (1),

$$\Delta\left(\frac{1}{r^{2n+1}}\right) = -(2n+1)\nabla\cdot\left(\frac{\mathbf{r}}{r^{2n+3}}\right)$$

$$= -(2n+1)\Big[\frac{\nabla\cdot\mathbf{r}}{r^{(2n+3)}} - (2n+3)\frac{\mathbf{r}\cdot\mathbf{r}}{r^{(2n+5)}}\Big].$$

Finally, using the facts that $\nabla\cdot\mathbf{r} = 3$ and $\mathbf{r}\cdot\mathbf{r} = r^2$, we conclude (3.20). □

Let us note the following obvious fact about homogeneous polynomials.

Lemma 4. *If $P_n(x,y,z)$ is a homogeneous polynomial of order n, then $r^2\boldsymbol{a}\cdot\nabla P_n$ is a homogeneous polynomial of order $n+1$ for any vector $\boldsymbol{a}\in\mathbb{R}^3$.*

Proof. It follows immediately from the fact that each component of ∇P_n is a homogeneous polynomial of degree $n-1$. □

We now introduce the following notation for directional derivatives in $\mathbb{R}^3$.

Definition 2. *For non-zero vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \cdots \boldsymbol{a}_n \in \mathbb{R}^3$, we write the* directional derivative *with respect to these vectors as,*

$$\frac{\partial^n}{\partial\boldsymbol{a}_1\partial\boldsymbol{a}_2\cdots\partial\boldsymbol{a}_n}(\cdot) := \boldsymbol{a}_1\cdot\nabla\left(\boldsymbol{a}_2\cdot\nabla\cdots\boldsymbol{a}_n\cdot\nabla\right)(\cdot).$$

The following proposition notes the relation between directional derivatives and homogeneous polynomials in $\mathbb{R}^3$.

Proposition 2. *For any non-zero vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \cdots \boldsymbol{a}_n \in \mathbb{R}^3$, there exists a homogeneous polynomial P_n such that*

$$\frac{\partial^n}{\partial \boldsymbol{a}_1 \partial \boldsymbol{a}_2 \cdots \partial \boldsymbol{a}_n}\left(\frac{1}{r}\right) = \frac{P_n}{r^{(2n+1)}}. \tag{3.21}$$

Proof. We use mathematical induction to show this result.

For $n = 1$ choose $\boldsymbol{a}_1 = (a_x, a_y, a_z)$. We then have,

$$\boldsymbol{a} \cdot \nabla\left(\frac{1}{r}\right) = -\boldsymbol{a} \cdot \frac{\mathbf{r}}{r^3} = -\frac{(a_x x + a_y y + a_z z)}{r^3},$$

in which case, $P_1 = -(a_x x + a_y y + a_z z)$.

We now proceed to show that the statement being true for some n implies that it is true for $n+1$. For $\boldsymbol{a}_{n+1} = \boldsymbol{a} := (a_x, a_y, a_z)$, consider

$$\boldsymbol{a} \cdot \nabla\left(\frac{P_n}{r^{(2n+1)}}\right) = \boldsymbol{a} \cdot \left[\frac{r^2 \nabla P_n - 2n P_n \mathbf{r}}{r^{2n+3}}\right].$$

Let us note that $(\boldsymbol{a} \cdot \mathbf{r}) P_n$ and $r^2 \nabla P_n \cdot \boldsymbol{a}$ are both homogeneous polynomials of degree $n+1$. So the $(n+1)^{th}$ derivative can be written as

$$\frac{\partial^n}{\partial \boldsymbol{a}_1 \partial \boldsymbol{a}_2 \cdots \partial \boldsymbol{a}_{n+1}}\left(\frac{1}{r}\right) = \frac{P_{n+1}}{r^{(2n+3)}}.$$

□

Proposition 3. *P_n defined by equation (3.21) is harmonic in $\mathbb{R}^3$. That is,*

$$\Delta P_n = 0. \tag{3.22}$$

Proof. For $\mathbf{r} \in \mathbb{R}^3 - \{\mathbf{0}\}$, let us note that $\Delta\left(\frac{1}{r}\right) = 0$. We then have,

$$\Delta \frac{\partial}{\partial x}\left(\frac{1}{r}\right) = \frac{\partial}{\partial x}\Delta\left(\frac{1}{r}\right) = 0.$$

Similarly,

$$\Delta \frac{\partial}{\partial y}\left(\frac{1}{r}\right) = 0, \ \Delta \frac{\partial}{\partial z}\left(\frac{1}{r}\right) = 0.$$

It then follows that

$$\Delta\left(\frac{\partial^n}{\partial \boldsymbol{a}_1 \partial \boldsymbol{a}_2 \cdots \partial \boldsymbol{a}_n}\left(\frac{1}{r}\right)\right) = 0.$$

Now using (3.21) of the previous proposition, we have

$$\Delta\left(\frac{P_n}{r^{(2n+1)}}\right) = 0$$

$$\Rightarrow \frac{1}{r^{2n+1}}\Delta P_n + 2\nabla P_n \cdot \nabla\left(\frac{1}{r^{2n+1}}\right) + P_n \Delta\left(\frac{1}{r^{2n+1}}\right) = 0.$$

Now using (3.19) and Euler's theorem on homogeneous functions: $\nabla P_n \cdot \mathbf{r} = nP_n$.

$$\Rightarrow \frac{1}{r^{2n+1}}\Delta P_n - \frac{2(2n+1)}{r^{2n+3}}(nP_n) + P_n \frac{2n(2n+1)}{r^{2n+3}} = 0.$$

Cancelling the last two terms in the previous equation, we conclude that on $\mathbb{R}^3 - \{\mathbf{0}\}$,

$$\Delta P_n = 0.$$

Using the smoothness of the polynomial P_n, the result holds true on $\mathbb{R}^3$. □

Corollary 2. $\frac{\partial^n}{\partial \boldsymbol{a}_1 \partial \boldsymbol{a}_2 \cdots \partial \boldsymbol{a}_n}\left(\frac{1}{r}\right)|_{r=1}$ *is a spherical harmonic of order* n.

Proof. By (3.21), we have

$$P_n = r^{2n+1}\frac{\partial^n}{\partial \boldsymbol{a}_1 \partial \boldsymbol{a}_2 \cdots \partial \boldsymbol{a}_n}\left(\frac{1}{r}\right).$$

Since by the previous proposition, P_n is harmonic on $\mathbb{R}^3$. Now using the observation (3.16), we conclude that $\frac{\partial^n}{\partial \boldsymbol{a}_1 \partial \boldsymbol{a}_2 \cdots \partial \boldsymbol{a}_n}\left(\frac{1}{r}\right)\Big|_{r=1}$ is a spherical harmonic. □

The uniqueness of the multipole expansion is called Sylvester's theorem. We direct the reader to Sylvester's paper for a proof.

Theorem 3 (Sylvester)**.** *Every spherical harmonic of order* n *can be written uniquely (up to reordering) as an* n^{th} *directional derivative of* $\frac{1}{r}$.

Proof. [59] □

3.3.3 Constructing Symmetric Spherical Harmonics

The most straightforward way to compute spherical harmonics of order l with symmetry Σ is to solve for coefficients c_{lm} that satisfy the property

$$\sum_{m=-l}^{l} c_{lm}\sigma(Y_{lm}) = \sum_{m=-l}^{l} c_{lm}Y_{lm}, \text{ for all } \sigma \in \Sigma,$$

where $\sigma(Y_{lm})$ represents the action of σ on Y_{lm}. In the previous equation, it is sufficient to only consider the generators of the group Σ. In either cases, determining the result of the action of σ on Y_{lm} can be algebraically quite tedious.

Instead of this brute force expansion, a more elegant approach has been taken by Poole [52], in which he constructs symmetric spherical harmonics using invariant operators. A related, but slightly different approach, based on invariant polynomials, has been developed by Hodgkinson [36] . Here, we summarize the method developed by Poole. This method is based on Sylvester's theorem, discussed above.

For any $Q \in O(3)$, we define the representation of $O(3)$ on real valued functions on $f : \mathbb{R}^3 \to \mathbb{R}$ by,

$$Qf(\mathbf{r}) := f(\boldsymbol{Q}^{\boldsymbol{T}}\mathbf{r}).$$

where $\mathbf{Q}$ is a 3-dimensional representation of $O(3)$ on $\mathbb{R}^3$.

Proposition 4. *For any* $\boldsymbol{Q} \in O(3)$,

$$Q\Big[\frac{\partial^n}{\partial \boldsymbol{a}_1 \partial \boldsymbol{a}_2 \cdots \partial \boldsymbol{a}_n}\left(\frac{1}{r}\right)\Big] = \frac{\partial^n}{\partial \boldsymbol{Q}^{\boldsymbol{T}}\boldsymbol{a}_1 \partial \boldsymbol{Q}^{\boldsymbol{T}}\boldsymbol{a}_2 \cdots \partial \boldsymbol{Q}^{\boldsymbol{T}}\boldsymbol{a}_n}\left(\frac{1}{r}\right). \tag{3.23}$$

Proof. For any $Q \in O(3)$,

$$Q\left(\frac{1}{r}\right) = Q\left(\frac{1}{|\mathbf{r}|}\right) = \frac{1}{|\mathbf{Q^T r}|} = \frac{1}{r}.$$

Now,

$$Q\left(\nabla f(\mathbf{r}) \cdot \boldsymbol{a}\right) = \nabla f(\boldsymbol{Q}^{\boldsymbol{T}}\boldsymbol{x}) \cdot \boldsymbol{Q}^{\boldsymbol{T}}\boldsymbol{a},$$

$$Q\left(\nabla\left(\frac{1}{r}\right)\cdot\boldsymbol{a}\right)=\nabla\left(\frac{1}{|\boldsymbol{Q^T}\mathbf{r}|}\right)\cdot\boldsymbol{Q^T a}=\boldsymbol{Q^T a}\cdot\nabla\left(\frac{1}{r}\right).$$

That is,

$$Q\frac{\partial}{\partial\boldsymbol{a}}\left(\frac{1}{r}\right)=\frac{\partial}{\partial\boldsymbol{Q^T a}}\left(\frac{1}{r}\right).$$

The result follows by repeating the argument for n vectors. □

It is clear from the preceding proposition that the symmetry of the spherical harmonic $\frac{\partial^n}{\partial\boldsymbol{a}_1\partial\boldsymbol{a}_2\cdots\partial\boldsymbol{a}_n}\left(\frac{1}{r}\right)$ is reflected by the symmetry of the set $\{\boldsymbol{a}_1,\boldsymbol{a_2},\cdots,\boldsymbol{a_n}\}\subset\mathbb{R}^3$. Therefore, we can construct spherical harmonics with an appropriate symmetry by constructing differential operators by suitably choosing the direction vectors $\boldsymbol{a}_i$ to reflect the symmetry in question. Sylvester's theorem guarantees the uniqueness of this expansion.

In what follows we only consider the exceptional subgroups of $O(3)$ as described in [23] to demonstrate Poole's procedure. These are the (achiral) tetrahedral ($\mathbb{T}\oplus\mathbb{Z}_2^c$), octahedral ($\mathbb{O}\oplus\mathbb{Z}_2^c$) and icosahedral ($\mathbb{I}\oplus\mathbb{Z}_2^c$) groups (these groups are defined below).

The following definition is introduced to simply notation in the discussion below,

$$\hat{x}=\frac{\partial}{\partial x},\ \hat{y}=\frac{\partial}{\partial y},\ \hat{z}=\frac{\partial}{\partial z}. \tag{3.24}$$

Tetrahedral Group:

The chiral tetrahedral group $\mathbb{T}$ is defined by the following presentation in terms of their generators,

$$\mathbb{T}=\langle s,t|s^2,\ t^3,\ (st)^3\rangle.$$

Recall that this means that $\mathbb{T}$ is a free group generated by s and t such that the following condition holds: $s^2=t^3=(st)^3=e$, where e is the identity element of the group.

Its representation on $\mathbb{R}^3$ can be realized by the following generators,

$$s = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, t = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

The symmetry group of a regular tetrahedron is the achiral tetrahedral group which contains the inversions through the origin,

$$-I = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

This group can be written as the direct sum: $\mathbb{T} \oplus Z_2^c$.

It is an easy check to verify that the following operators are invariant under the (achiral) tetrahedral group with respect to the action defined above,

$$L := \hat{z}\hat{y}\hat{x}, \tag{3.25a}$$

$$M := \hat{x}^2\hat{y}^2 + \hat{y}^2\hat{z}^2 + \hat{z}^2\hat{x}^2. \tag{3.25b}$$

For instance,

$$sL = (\hat{z})(-\hat{y})(-\hat{x}) = \hat{z}\hat{y}\hat{x} = L,$$

$$tL = (\hat{x})(\hat{z})(\hat{y}) = \hat{z}\hat{y}\hat{x} = L.$$

Similarly, it follows that,

$$sM = M,$$

$$tM = M.$$

As a consequence of Sylvester's theorem, any spherical harmonic of order l that is invariant under $\mathbb{T}$ can be written uniquely (up to reordering) as follows,

$$\sum_{3p+4q=l,\ p,q\in\mathbb{Z}} L^p M^q \left(\frac{1}{r}\right)\Big|_{r=1}. \tag{3.26}$$

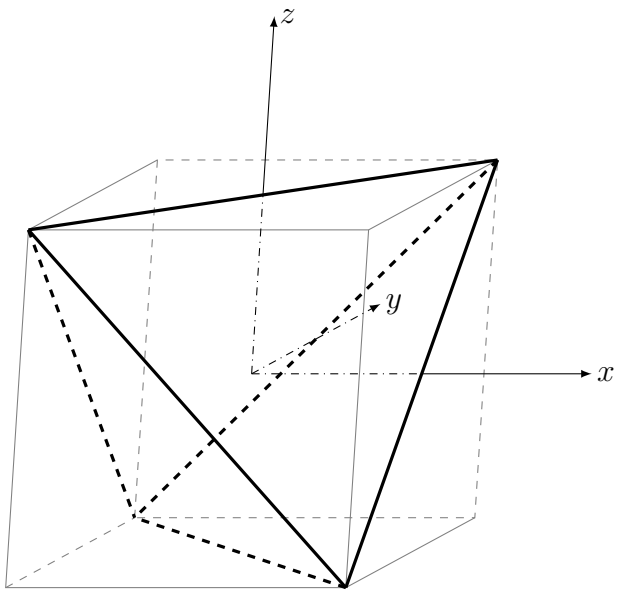


Figure 3.1: Regular tetrahedron

For example, if we choose $l = 3$, the tetrahedrally symmetric spherical harmonic of order 3 is

$$Y_3^{\mathbb{T}\oplus\mathbb{Z}_2^c} = L\left(\frac{1}{r}\right)\Big|_{r=1}.$$

Octahedral Group

The octahedral group $\mathbb{O}$ is a supergroup of $\mathbb{T}$ with the following presentation:

$$\mathbb{O} = \langle a, b | a^2,\ b^3,\ (ab)^4 \rangle.$$

Its representation on $\mathbb{R}^3$ can be realized by the following generators,

$$a = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, b = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

We obtain the achiral octahedral group, the symmetry of a regular octahedron, by including the group of reflections through the origin, *i.e.*, via the direct sum, $\mathbb{O} \oplus \mathbb{Z}_2^c$.

It can be checked that the operators L^2 and M are invariant under the (achiral) octahedral group. These operators can be used to construct octahedrally invariant spherical harmonics using following expansion,

$$Y_l^{\mathbb{O}\oplus\mathbb{Z}_2^c} = \sum_{6p+4q=l,\ p,q\in\mathbb{Z}} L^{2p} M^q \left(\frac{1}{r}\right)\Big|_{r=1}. \tag{3.27}$$

We proceed to relate the octahedrally symmetric spherical harmonic described abstractly in the preceding equation in terms of the familiar spherical harmonics, Y_{lm}.

We introduce the following two definitions,

$$\hat{\xi} := \Big(\hat{x} - i\hat{y}\Big), \tag{3.28a}$$

$$\hat{\eta} := \Big(\hat{x} + i\hat{y}\Big). \tag{3.28b}$$

Therefore, we have,

$$4\hat{x}\hat{y} = i\Big(\hat{\xi} + \hat{\eta}\Big)\Big(\hat{\xi} - \hat{\eta}\Big) = i(\hat{\xi}^2 - \hat{\eta}^2).$$

Let us also note that,

$$\hat{x}^2 + \hat{y}^2 = \hat{\xi}\hat{\eta}.$$

Since,

$$(\hat{x}^2 + \hat{y}^2 + \hat{z}^2)\Big(\frac{1}{r}\Big) = 0,$$

the following equation follows,

$$\hat{\xi}\hat{\eta}\Big(\frac{1}{r}\Big) = (\hat{x}^2 + \hat{y}^2)\Big(\frac{1}{r}\Big) = -\hat{z}^2\Big(\frac{1}{r}\Big).$$

For example, for $l = 4$, the only allowed choice for p and q in (3.27) is: $p = 0$ and $q = 1$. Therefore, the octahedrally invariant spherical harmonic of order 6 can be written as,

$$M\Big(\frac{1}{r}\Big)\Big|_{r=1}.$$

That is, we have,

$$\begin{aligned} M\Big(\frac{1}{r}\Big) &= -\frac{1}{16}(\hat{\xi}^2 - \hat{\eta}^2)^2\Big(\frac{1}{r}\Big) + \hat{z}^2(\hat{x}^2 + \hat{y}^2)\Big(\frac{1}{r}\Big) \\ &= -\frac{1}{16}(\hat{\xi}^4 + \hat{\eta}^4 - 2\hat{\xi}^2\hat{\eta}^2)\Big(\frac{1}{r}\Big) - \hat{z}^4\Big(\frac{1}{r}\Big) \\ &= -\frac{1}{16}(\hat{\xi}^4 + \hat{\eta}^4)\Big(\frac{1}{r}\Big) - \frac{7}{8}\hat{z}^4\Big(\frac{1}{r}\Big) \\ &= -\frac{1}{8}Y_{44} - \frac{7}{8}4!Y_{40} \\ &= -\frac{1}{8}\Big(Y_{44} + 168Y_{40}\Big), \end{aligned}$$

where we have used the following facts (from Hobson's classic text [35], pgs. 134-135)[1] in the steps above to replace the directional derivatives $\hat{\xi}$, $\hat{\eta}$ and $\hat{z}$ in terms of the familiar spherical harmonics,

$$\hat{z}^{(n-m)}(\hat{\xi}^m + \hat{\eta}^m)\left(\frac{1}{r}\right)\Big|_{r=1} = (-1)^{n-m}2(n-m)!Y_{nm}, \tag{3.29}$$

$$\hat{z}^n\left(\frac{1}{r}\right)\Big|_{r=1} = (-1)^n n!Y_n, \tag{3.30}$$

Icosahedral Group

The (chiral) icosahedral group has the following presentation

$$\mathbb{I} = \langle c, d | c^2,\ d^3,\ (cd)^5 \rangle.$$

Its representation in $\mathbb{R}^3$ can be realized with the following matrices,

$$c = \begin{pmatrix} -\frac{\tau}{2} & \frac{1}{2\tau} & \frac{1}{2} \\ \frac{1}{2\tau} & -\frac{1}{2} & \frac{\tau}{2} \\ \frac{1}{2} & \frac{\tau}{2} & \frac{1}{2\tau} \end{pmatrix}, d = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

[1] We have modified the normalization to be consistent with definitions (3.28)

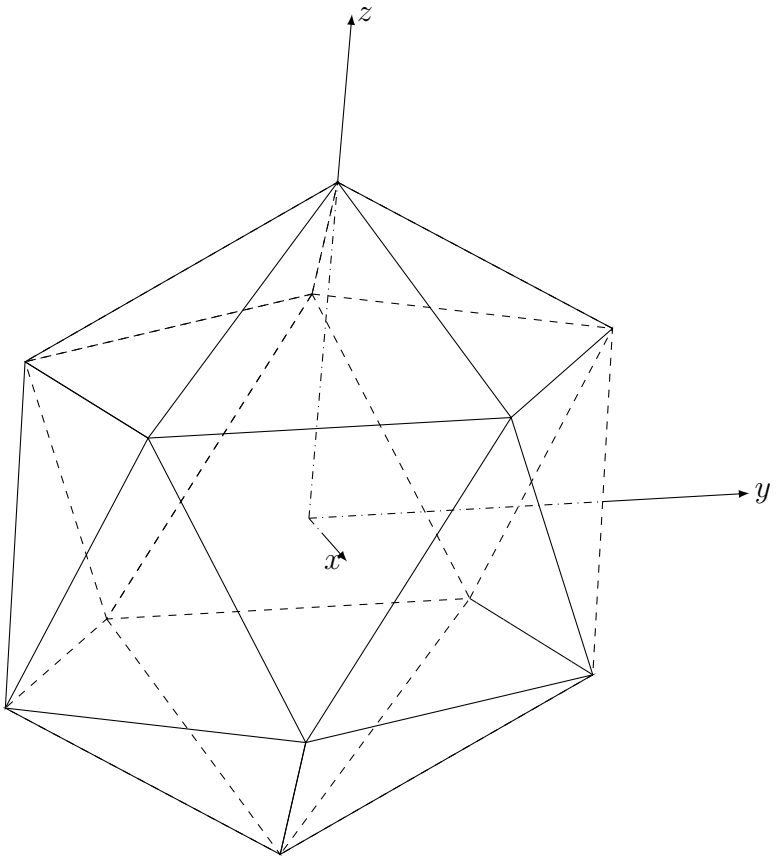


Figure 3.2: Regular Icosahedron

It can be shown that [52] the following operators are invariant under the achiral icosahedral group $\mathbb{I} \oplus \mathbb{Z}_2^c$,

$$P = \hat{z}(\hat{\xi}^5 + \hat{\eta}^5) + 11\hat{z}^6,$$

$$Q = \hat{\xi}^{10} + \hat{\eta}^{10} - 228\hat{z}^5(\hat{\xi}^5 + \hat{\xi}^5) + 494\hat{z}^{10}.$$

Using the same argument presented in the previous two subgroup, an icosahedrally symmetric spherical harmonic of order l can be constructed using the operators P and Q as follows,

$$Y_l^{\mathbb{I}\oplus\mathbb{Z}_2^c} = \sum_{6p+10q=l,\ p,q\in\mathbb{Z}} P^p Q^q \left(\frac{1}{r}\right)\Big|_{r=1}. \tag{3.31}$$

For $l = 6$, this is only possible for $p = 1$ and $q = 0$. We have,

$$\begin{aligned} Y_6^{\mathbb{I}\oplus\mathbb{Z}_2^c} &= P\left(\frac{1}{r}\right)\Big|_{r=1} \\ &= \left[\hat{z}(\hat{\xi}^5 + \hat{\eta}^5) + 11\hat{z}^6\right]\left(\frac{1}{r}\right)\Big|_{r=1} \\ &= -2Y_{65} + 11 \cdot 6! Y_{60} \\ &= -2Y_{65} + 7,920 Y_{60}. \end{aligned}$$

A similar procedure when applied to the case $l = 10$ gives us,

$$\begin{aligned} Y_{10}^{\mathbb{I}\oplus\mathbb{Z}_2^c} &= 2Y_{10,10} + 1,792,627,200 Y_{10,0} + 54,720 Y_{10,5} \\ &= 2\Big(Y_{10,10} + 896,313,600 Y_{10,0} + 27,360 Y_{10,5}\Big). \end{aligned}$$

CHAPTER 4

SECOND VARIATION AND STABILITY

4.1 Introduction

The main theme of this chapter is the question of stability of equilibria. It might seem straightforward that to determine stability, one has to check for the positive definiteness of the second variation. However, due to the constraints involved in the problem, checking for stability is a bit more delicate. For constrained problems, an equilibrium solution is considered stable if the second variation is positive definite for all variations that respect the linearized constraint equations. In this way, the stability of solutions is intimately tied to the constraints imposed on the system.

In chapter (2), we saw that local (LA) and global (GA) area formulations yield same solutions sets (up to reparametrization) and therefore were equivalent formulations. However, it is not obvious if the two formulations agree on matters of stability. In this chapter we focus on resolving this issue. We shall show that for (oriented) surfaces of genus zero, both the formulations yield identical stability criteria and therefore are truly equivalent formulations.

4.2 Stability, Hessian and Constraints

Stability of a system crucially depends on the dynamics of the system. The true dynamics of the lipid-membrane problem is quite complex. So, the best one could do in this case is to assume some form of a dissipative dynamics. By using a Lyapunov notion of stability, a solution $(\mathbf{x}^*, \phi^*)$ to the system (2.30) is considered stable if the associated Hessian is positive definite for all possible *admissible variations*.

For constrained systems, a variation is considered *admissible* if it satisfies the linearized constraint equations. Therefore, the stability of the system is dependent on the constraints imposed. But this poses the following question - should area constraint be assumed to be local (LA formulation) or global (GA formulation)? We have seen in section (2.6) the equivalence of the two formulations for compact genus zero surfaces with respect to determination of equilibria. We shall see later in this chapter that under the same assumption, both the area constraints give identical stability criteria.

4.2.1 Linearized Constraints and Admissible Variations

To define admissible variations for the two formulations, we first linearize both the area constraints.

The linearization of the local area constraint , (2.7),

$$J = 1, \tag{4.1}$$

is given by

$$(\nabla \cdot \mathbf{v} - 2Hw) = 0. \tag{4.2}$$

Variations $(\mathbf{v}, w)$ are considered *admissible for the LA formulation* if they satisfy the previous equation.

On the other hand the linearization of the global area constraint, (2.5),

$$\int_{S^2} (J - 1)\, dA = 0, \tag{4.3}$$

is given by

$$\int_{\omega} (\nabla \cdot \mathbf{v} - 2Hw)\, da = 0. \tag{4.4}$$

This may be further simplified by using the divergence theorem,

$$\int_{\omega} Hw\, da = 0. \tag{4.5}$$

We consider variations $(\mathbf{v}, w)$ to be *admissible for the GA formulation* if they satisfy the preceding equation. Note that the tangential variations, $\mathbf{v}$, vanishes from the linearization of the global area constraint.

It is clear that equations (4.2) and (4.5) give two very different criteria for admissible variations. We shall proceed to show the equivalence of these criteria and therefore the equivalence of the LA and GA formulations for stability. For this we use tools from Hodge theory that we briefly summarize in the next section.

4.3 Hodge Theory

In this section we briefly summarize the main results of Hodge theory in the context of Riemannian manifolds. In what follows, (ω, g) stands for a Riemannian manifold ω of dimension n with a metric $g_{\alpha\beta}dx^{\alpha}dx^{\beta}$. More details can be found in [64, 21]. No originality is claimed in this section.

4.3.1 Codifferential and the Laplace-Beltrami Operator

The Hodge star operator $(*)$ formalizes the duality between the space of p forms and $n-p$ forms on ω. Let us write a p form on ω in local coordinates,

$$\alpha = \alpha_{k1\cdots k_p} dx^1 \wedge \cdots dx^p.$$

We define the *Hodge dual of* α as follows,

Definition 3 (Hodge Dual)**.** *For every p-form α, on an n-Riemannian manifold (ω, g), there is a $(n-p)$ form that is defined (in local coordinates) by*

$$*\alpha := \alpha^*_{j_1\cdots j_{n-p}} dx^1 \wedge dx^2 \wedge \cdots \wedge dx^{n-p},$$

the coefficients being given by,

$$\alpha^*_{j_1\cdots j_{n-p}} = \sqrt{g} \sum_{k1<\cdots<k_p} \alpha^{k_1\cdots k_p} \epsilon_{k_1\cdots k_p j_1\cdots j_{n-p}},$$

where

$$\alpha^{k\cdots r} = g^{ks}\cdots g^{rt}\alpha_{s\cdots t},$$

and $\epsilon_{k1\cdots k_p j_1\cdots j_{n-p}}$ *is the* n *dimensional Levi-Civita symbol.*

The following properties follow from the definition,

1. $** = (-1)^{p(n-p)}$.
2. $*1 = \sqrt{g}\epsilon_{12\cdots n}dx^1 \wedge \cdots \wedge dx^n$ is the volume form on ω.
3. For any function f and a p-form α, $*(f\alpha) = f(*\alpha)$.

We now proceed to show that the usual divergence and Laplace-Beltrami operators of vector calculus can be written in terms of the Hodge star operator.

Definition 4. *For every vector field* $\mathbf{v} = v^\alpha \boldsymbol{\partial}_\alpha$ *(expressed explicitly in terms of its basis,* $\boldsymbol{\partial}_\alpha$*), there is a 1-form* $v^\flat$*, defined by,*

$$v^\flat := v_\beta dx^\beta,$$

where $v_\beta = v^\alpha g_{\alpha\beta}$.

Proposition 5. *For any vector field* $\mathbf{v}$ *on a 2-manifold* ω*, the divergence can be expressed as follows*

$$\nabla \cdot \mathbf{v} = *d * v^\flat. \tag{4.6}$$

Proof. In local coordinates we write,$\mathbf{v} = v^\alpha \boldsymbol{\partial}_\alpha$, where $\boldsymbol{\partial}_\alpha$ is the tangential basis vectors. From the previous definition, we have,

$$v^\flat = g_{\alpha\beta}v^\alpha dx^\beta.$$

Expanding the right hand side of (4.6),

$$*d * v^\flat = *d\Big(\sqrt{g}g^{\beta\gamma}g_{\alpha\beta}\epsilon_{\gamma\delta}v^\alpha\, dx^\delta\Big)$$

$$= *\Big[\partial_\beta\Big(\sqrt{g}v^\alpha\Big)\epsilon_{\alpha\delta}dx^\beta \wedge dx^\delta\Big]$$
$$= \frac{1}{\sqrt{g}}\partial_\alpha\Big(\sqrt{g}v^\alpha\Big) = \nabla \cdot \mathbf{v},$$

where the last equality follows from the definition of divergence in curvilinear coordinates (in terms of the metric tensor). □

The Hodge star can be used to define the *codifferential* operator,

Definition 5 (Codifferential)**.** *The codifferential δ is a linear operator that takes p forms to $(p-1)$ forms and is defined*[1] *by*

$$\delta = (-1)^{n(p+1)} * d*,$$

and for a 0-form (real valued function on the manifold) f, $\delta f \equiv 0$.

The notion of a Laplace-Beltrami operator can now be extended to act on p-forms using the following definition,

Definition 6 (Laplace-Beltrami)**.** *The Laplace-Beltrami operator on p-forms is defined by*

$$\Delta = \delta d + d\delta. \tag{4.7}$$

Let us make a connection between the Laplace-Beltrami defined by (4.7) with the operator expressed via the metric $g_{\alpha\beta}$, in the case when restricted to 0-forms on 2-manifolds, i.e., functions on 2-manifolds.

Proposition 6. *For any scalar function $f : \omega \to \mathbb{R}$, on a 2-manifold ω,*

$$\Delta f = \frac{1}{\sqrt{g}}\partial_\alpha\left(\sqrt{g}g^{\alpha\beta}\partial_\beta f\right).$$

[1]Most books define codifferential to be the negative of what is defined above. The choice here is motivated by maintaining a consistent definition for the Laplace-Beltrami operator

Proof. Let us first recall that for a scalar function $f : \omega \to \mathbb{R}$, $\delta f \equiv 0$. Therefore,

$$\Delta f = \delta df$$

$$= \delta \left(\partial_\alpha f dX^\alpha \right)$$

$$= (-1)^{2n} * d * \left(\partial_\alpha f dX^\alpha \right)$$

$$= *d \left(\sqrt{g} \epsilon_{\alpha\beta} \partial^\beta f dX^\alpha \right)$$

$$= * \left(\partial_\gamma \left(\sqrt{g} \partial^\beta f \right) \epsilon_{\alpha\beta} dX^\gamma \wedge dX^\alpha \right)$$

$$= \partial_\gamma \left(\sqrt{g} \partial^\beta f \right) \epsilon_{\alpha\beta} * \left(dX^\gamma \wedge dX^\alpha \right) = \frac{1}{\sqrt{g}} \partial_\alpha \left(\sqrt{g} \partial^\alpha f \right).$$

□

The Hodge star can also be used to define an innerproduct on $\Lambda^p(\omega)$, the space of p-forms on ω.

Definition 7 (Innerproduct of p-forms)**.** *For any two p-forms α,$\beta \in \Lambda^p(\omega)$, their innerproduct is defined by*

$$\langle \alpha, \beta \rangle = \int_\omega \alpha \wedge *\beta.$$

The innerproduct may further be extended to $\Lambda(\omega) := \bigoplus \Lambda^p(\omega)$, the space of all possible forms on ω, by requiring $\Lambda^p(\omega)$ to be orthogonal $\Lambda^q(\omega)$ for all $0 \leq p \neq q \leq n$.

The following results immediately follow [64],

Proposition 7. *δ is the adjoint of d on $\Lambda(\omega)$. That is,*

$$\langle d\alpha, \beta \rangle = \langle \alpha, \delta\beta \rangle,$$

for forms α, β in $\Lambda(\omega)$.

Proof. It is sufficient to consider the case when $\alpha \in \Lambda^{p-1}(\omega)$ and $\beta \in \Lambda^p(\omega)$. The general case follows from the linearity of d and orthogonality of $\Lambda^p(\omega)$ in $\Lambda(\omega)$.

$$d(\alpha \wedge *\beta) = d\alpha \wedge *\beta + (-1)^{p-1}\alpha \wedge d * \beta$$

$$= d\alpha \wedge *\beta - \alpha \wedge *\delta\beta.$$

Integrating both sides over ω and using the Stokes' theorem [10], we obtain

$$0 = \int_\omega (d\alpha \wedge *\beta - \alpha \wedge *\delta\beta) = \langle d\alpha, \beta\rangle - \langle \alpha, \delta\beta\rangle.$$

Thus,

$$\langle d\alpha, \beta\rangle = \langle \alpha, \delta\beta\rangle.$$

□

Corollary 3. Δ *is self-adjoint. That is,*

$$\langle \Delta\alpha, \beta\rangle = \langle \alpha, \Delta\beta\rangle$$

for every $\alpha, \beta \in \Lambda^p(\omega)$.

Proposition 8. $\Delta\alpha = 0$ *iff* $d\alpha = 0$ *and* $\delta\alpha = 0$.

Proof. Clearly, if $d\alpha = 0$ and $\delta\alpha = 0$ the it follows form the definition that $\Delta\alpha = 0$.

For the converse, consider

$$\langle \Delta\alpha, \alpha\rangle = \langle (d\delta + \delta d)\alpha, \alpha\rangle$$

$$= \langle \delta\alpha, \delta\alpha\rangle + \langle d\alpha, d\alpha\rangle.$$

Thus, if $\Delta\alpha = 0$, it follows that $d\alpha = 0$ and $\delta\alpha = 0$. □

The following corollary immediately follows.

Corollary 4. *The only harmonic functions $\Delta f = 0$ on a compact, connected, oriented, Riemannian manifold are the constant functions.*

The idea of harmonic functions can be generalized to p-forms by the following definition,

Definition 8 (Harmonic Forms)**.** *A p-form α is said to be* harmonic *if it satisfies*

$$\Delta\alpha = 0.$$

4.3.2 Hodge Decomposition

Consider a smooth vector field, $\mathbf{V}$ in $\mathbb{R}^3$. It is well known [2] that the vector field may be decomposed via the Helmholtz decomposition in terms of curl free and divergence free components. That is, there exist scalar field, φ, and a vector field, $\mathbf{A}$, such that

$$\mathbf{V} = \nabla\varphi + \nabla \times \mathbf{A}.$$

Hodge decomposition is a generalization of this idea to vectors fields on manifolds.

Theorem 4 (Hodge Decomposition Theorem)**.** *For every $0 \leq p \leq n$, any p-form α has the following decomposition*

$$\alpha = d\sigma + \delta\tau + \omega, \tag{4.8}$$

where σ and τ are $p-1$ and $p+1$ forms respectively, and ω is a harmonic p-form. Moreover, this decomposition is orthogonal, i.e,

$$\langle d\sigma, \delta\tau\rangle = \langle d\sigma, \omega\rangle = 0. \tag{4.9}$$

An important consequence of the Hodge theorem is the following result which relates the de Rahm cohomology to the space of harmonic forms.

Theorem 5. *Each de Rham cohomology class on a compact Riemannian manifold contains a unique harmonic representative.*

The proof of the previous theorems can be found in [21, 64].

4.4 Equivalence of Local and Global Area Constraints

For every tangent field $\mathbf{v}$ of a 2-manifold, let us consider the associated 1-form, $v^\flat$. By Hodge decomposition, we have the following,

$$v^\flat = d\sigma + \delta\tau + \eta, \tag{4.10}$$

where σ is a 0-form (function), τ is a 2-form and η is a 1-harmonic form. For genus zero surfaces, it is well known that the first de Rahm cohomology is trivial [10]. That is, all the closed forms are exact. Using this fact and theorem (5), we can conclude that the harmonic 1-form η is an exact form. By absorbing this exact form into $d\sigma$ in (4.10), we can rewrite the equation as,

$$v^\flat = d\sigma + \delta\tau. \tag{4.11}$$

Note that for a 2-manifold for any vector field $\mathbf{v}$,

$$\nabla \cdot \mathbf{v} = *d * v^\flat. \tag{4.12}$$

Using the decomposition, (4.11) in the previous equation,

$$\nabla \cdot \mathbf{v} = *d * (d\sigma + \delta\tau). \tag{4.13}$$

Now using the fact that $*d* = \delta$ for 2-manifolds, we get

$$\nabla \cdot \mathbf{v} = \delta d\sigma = \Delta\sigma, \tag{4.14}$$

where we have used the facts that $\delta^2 = 0$ and $\delta\sigma = 0$.

Recall the linearized local area constraint (4.2),

$$\nabla \cdot \mathbf{v} = 2Hw. \tag{4.15}$$

If we now use (4.14), we get the following equivalent condition for the linearized local are constraint,

$$\Delta\sigma = 2Hw. \tag{4.16}$$

From the existence theory of elliptic PDE [64, 17], we have that the previous equation has a solution if and only if $2Hw$ is orthogonal to the null space of of the adjoint operator $\Delta\cdot$. Using the self-adjointness of Δ (cf. Cor. 3)), and the fact that the only harmonic functions on a compact oriented Riemannian manifold are constant functions (cf. corollary (4)), we conclude

$$\nabla \cdot \mathbf{v} = 2Hw \iff \int_\omega 2Hw \, da = 0. \tag{4.17}$$

We have thus established the following theorem:

Theorem 6. *The set of admissible variations for the LA formulation is identical to the set of admissible variations for the GA formulation. Since the second variation (summarized below) is also identical for both formulations, their equivalence for stability follows.*

4.5 Second Variation

For any equilibrium solution $(\mathbf{x}^*, \phi^*)$, we compute the second variation,

$$\mathcal{H}(\mathbf{x}^*, \phi^*)[w, \mathbf{v}, \psi] = \delta^2\mathcal{E}(\mathbf{x}^*, \phi^*) = \frac{d}{d\alpha}\delta\mathcal{E}\Big(\mathbf{x}^* + \alpha(\mathbf{v} + w\mathbf{n}), \phi^* + \alpha(\psi + \nabla\phi \cdot \mathbf{v})\Big)\Big|_{\alpha=0}, \tag{4.18}$$

where w, $\mathbf{v}$, ψ are the variations in the normal, tangential directions and the concentration variables, respectively, as seen in chapter (2).

The detailed calculations are presented in the appendix (C). For our present purposes it suffices to note the following two important observations (1) both the LA and the GA formulations yield the same expression for the second variation and (2) all the terms involving the tangential variation, $\mathbf{v}$, vanishes from the second variation and it takes the following form,

$$\mathcal{H}[w,\psi] = \int_\omega H_1[w,w] + H_2[w,\psi] + H_3[\psi,\psi]\, da, \tag{4.19}$$

where H_1, H_2 and H_3 are symmetric bilinear operators on their respective arguments given by

$$\begin{aligned} H_1 = \frac{c}{2}(\Delta w)^2 + [c(5H^2 - K) - \tilde{\gamma} + \Delta c_g] w\Delta w + \Big[\epsilon\phi^\alpha\phi^\beta - 2Hc\tilde{b}^{\alpha\beta} - \nabla^{\alpha\beta}c_g\Big] w\nabla_{\alpha\beta}w \\ + 2\Big[H\nabla^\alpha(cH) - b^{\alpha\beta}(cH)_\beta - \frac{K}{2}\nabla^\alpha c_g\Big] w\nabla_\alpha w \\ + \Big[2\tilde{\gamma}K + c(8H^4 - 10H^2K + 2K^2) + 2\epsilon H b^{\alpha\beta}\phi_\alpha\phi_\beta - 3\epsilon K\phi_\alpha\phi^\alpha + 2Hp\Big] w^2, \end{aligned} \tag{4.20a}$$

$$\begin{aligned} H_2 = 2\Big\{-2\epsilon\left[\nabla_\alpha(b^{\alpha\beta}w\phi_\beta) - \nabla^\alpha(Hw)\phi_\alpha\right] + c'H\Big[\Delta w + 2(2H^2 - K)w\Big] + \\ c'_g\left[\tilde{b}^{\alpha\beta}\nabla_{\alpha\beta}w + 2KHw\right]\Big\}\psi, \end{aligned} \tag{4.20b}$$

$$H_3 = -\epsilon\psi\Delta\psi + (W'' + c''H^2 + c''_gK)\psi^2, \tag{4.20c}$$

where the variations w and ψ satisfy the following constraints,

$$\int_\omega Hw\, da = 0, \tag{4.21}$$

$$\int_\omega [\psi - 2H\phi w]\, da = 0. \tag{4.22}$$

Note that due to the equivalence established in theorem (6), we use the linearized global area constraint above.

4.6 Volume Control

By volume control, we mean, fixing the volume enclosed by the vesicle. This is done by enforcing the constraint that the enclosed volume V has a fixed prescribed value V_0,

$$V = V_0. \tag{4.23}$$

Volume control is a hard loading device and the interior pressure is constitutively an undetermined Lagrange multiplier. The need for fixing volume is not very obvious. It is mainly motivated by our computational results discussed in chapter (8). We find that without volume control, it is not possible to get stable pinched solutions (that are observed experimentally).

We emphasize that we do not impose volume control for computing equilibria. In fact doing so would be infeasible because the trivial spherical homogeneous state is an equilibrium solution for arbitrary pressure, reflective of the incompressibility of the membrane. This inherent nonuniquness for pressure makes continuation on the trivial branch impossible with volume control. The trivial branch would be degenerate and every point on it would be a bifurcation point with respect to modes that are spherical but correspond to a different internal pressure.

4.6.1 Linearization and Local Stability

Although volume control is not very convenient for computations due to the degenerate trivial branch, the local stability of the branch with respect to volume control can be determined by checking if the modes satisfy the linearization of the volume constraint,

$$\int_\omega w \, da = 0. \tag{4.24}$$

That is, with volume control included, variations $(\mathbf{v}, w)$ are considered admis-

sible if they satisfy (4.21), (4.22) and (4.24). As noted above, in computational results summarized in chapter 8, we find stable branches only when we impose volume control.

CHAPTER 5

GAUGE SYMMETRY AND GAUGE FIXING

5.1 Introduction

Fluidity of lipid membrane manifests as reparametrization symmetry of the energy. That is, the energy is invariant under reparametrization. We saw in chapter (2) that this symmetry leads to a redundancy in the Euler-Lagrange equations, where there are fewer equations than unknowns. It further leads to an infinite dimensional null space for the hessian (about any equilibrium solution). Both these features pose considerable challenges to numerical computation of equilibria, their stability and for establishing rigorous analytical results for the model.

Most important theories of physics are described via Lagrangians that are invariant under a particular symmetry group. Such physical theories are called *gauge theories* and the associated symmetry as *gauge symmetry*. In this chapter we borrow these ideas from physics literature [22] and view the lipid membrane system with its reparametrization symmetry as an example of a gauge theory. Gauge symmetry leads to the system having redundant degrees of freedom called *gauge freedom*. The redundancy in the Euler-Lagrange equations noted above is due to gauge freedom inherent to the system. A simplest example of a gauge theory is potential theory where the gauge freedom is the arbitrariness in the choice of the datum for the potential energy. A simple, yet, nontrivial example is Maxwell's theory of electromagnetism. The gauge freedom, here, is the liberty to add gradient of an arbitrary scalar function and curl of an arbitrary vector field to the scalar and vector potentials, respectively.

Yet another example is Einstein's General Theory of Relativity(GR) [51] which has reparametrization invariance as its gauge symmetry. Gauge fixing is GR is

done using a variety of gauges [56, 34, 58] but the "harmonic gauge" is the most popular gauge[58] used. In this chapter, we use GR as a guiding principle in our search for a gauge fixing procedure to the lipid membrane problem.

5.2 Gauge Symmetry and Gauge Fixing Procedures

The simplest example of gauge symmetry as noted in the introduction occurs in newtonian potential theory. Recall that for a given potential energy $\psi(\mathbf{x})$ of a particle $\mathbf{x}$ with mass m, the dynamics is governed by

$$m\frac{d^2\mathbf{x}}{dt^2} = \nabla\psi(\mathbf{x}).$$

Since a constant translate of the potential energy, $\psi(\mathbf{x})+c$ also leads to the same dynamics, there is a freedom to choose the datum, c, for the potential energy. This is the gauge freedom for this theory. Intuitively this freedom can be understood by noting that only the *difference in energy* is a measurable quantity. Therefore, the easiest way to break this gauge symmetry is by arbitrarily fixing the constant c.

We shall now provide two nontrivial examples of gauge symmetry that are found in classical physics - Maxwell's electromagnetic theory and Einstein's theory of General Relativity.

5.2.1 Maxwell's Equations

Maxwell's equations [47] for the electric and magnetic field in vacuum can be written as follows,

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \quad \nabla \cdot \mathbf{B} = 0, \tag{5.1}$$

$$\nabla \cdot \mathbf{E} = 0, \quad \nabla \times \mathbf{B} = \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}, \tag{5.2}$$

where $\mathbf{E}$ and $\mathbf{B}$ are the electric and magnetic fields respectively and c, the speed of light in vacuum.

In the potential formulation of Maxwell's laws, the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ are expressed in terms of scalar and vector potentials φ and $\mathbf{A}$ as,

$$\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}. \tag{5.3}$$

With this choice, equations (5.1) are automatically satisfied. However equations (5.3) do not uniquely determine the fields. The following choice for the scalar and vector potentials,

$$\varphi' = \varphi - \frac{\partial \chi}{\partial t}, \quad \mathbf{A}' = \mathbf{A} + \nabla\chi, \tag{5.4}$$

where $\chi(\mathbf{x}, t)$ is any (smooth) scalar function on $\mathbb{R}^3$, also satisfy equations (5.3) and therefore the Maxwell's equations. This follows from the observation that curl of a gradient and divergence of a curl are both identically zero. Therefore, the scalar and vector potentials can only be determined up to a scalar function χ. This nonuniqueness in the choice of φ and $\mathbf{A}$ may be reconciled by noting that the electric and magnetic fields are the true observables of nature[1] which is not the case for potentials. They are just a convenient mathematical tool.

As a result of this gauge freedom, it is impossible to solve Maxwell's equations uniquely, when expressed in terms of $(\varphi, \mathbf{A})$. Since, all solutions can only be determined up to an arbitrary function χ. The standard way to get around this redundancy is to perform a *gauge fixing* procedure in which an extra equation is supplemented to the Maxwell's equations. The equation is chosen such that the gauge symmetry expressed in (5.4) is either partially or completely broken. A wide range of possibilities have been suggested, for example,

$$\text{Coulomb Gauge: } \nabla \cdot \mathbf{A} = 0,$$

[1]This is not true in Quantum Field Theory, see Aharanov-Bohm effect [20]

$$\text{Lorenz Gauge: } \frac{1}{c^2}\frac{\partial \varphi}{\partial t} + \nabla \cdot \mathbf{A} = 0,$$

$$\text{Weyl Gauge: } \varphi = 0.$$

It is important to note that all these gauges are *incomplete*, in the sense that they do not completely break the gauge symmetry. They do not constrain the arbitrariness in the choice of χ completely. Their use lies primarily in the simplifications they provide to the Maxwell's equations. For example, the wave nature of the electromagnetic field can be immediately inferred when Maxwell's equations, (5.2) are written in the Lorenz gauge,

$$\frac{1}{c^2}\frac{\partial^2 \varphi}{\partial t^2} - \Delta \varphi = 0,$$

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} - \Delta \mathbf{A} = \mathbf{0}.$$

5.2.2 General Relativity

Einstein's General Relativity (GR) is an other example of a gauge theory. The relevance of this example to the lipid membrane problem lies in the fact that both the theories have the same gauge symmetry, namely, reparametrization invariance. Due to this similarity, we use the procedure of gauge fixing in GR as motivation in the search for an appropriate procedure for the lipid membrane problem.

In GR, space-time is considered to be a four dimensional pseudo-Riemannian manifold and the fundamental quantity of interest is its metric tensor[2], $g_{\alpha\beta}$. Einstein's field equations are a set of partial differential equations for the metric tensor written as follows,

$$G_{\mu\nu} + g_{\mu\nu}\Lambda = \frac{8\pi G}{c^4} T_{\mu\nu}, \quad \mu, \nu \in \{0, 1, 2, 3\}, \tag{5.5}$$

[2]In this section $\alpha, \beta \in \{0, 1, 2, 3\}$, where $x^0 = t$, $x^1 = x$, $x^2 = y$ and $x^3 = z$

where $G_{\mu\nu}$ is the Einstein curvature tensor (defined below), Λ is the cosmological constant, G is the gravitational constant, c, the speed of light in vacuum and $T_{\mu\nu}$, the stress-energy tensor.

The Einstein curvature tensor is defined using the Ricci tensor $R_{\mu\nu}$ as follows,

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R.$$

The Ricci curvature tensor being the contraction of the Riemann curvature tensor,

$$R_{\mu\nu} = R^{\alpha}_{\mu\alpha\nu}. \tag{5.6}$$

The scalar curvature, R, is the contraction of the Ricci curvature,

$$R = R^{\mu}_{\mu}. \tag{5.7}$$

The tensors $R_{\mu\nu}$, $g_{\mu\nu}$ and $T_{\mu\nu}$ are all symmetric. Thus, equation (5.5) only contain ten independent equations. However, four of the ten equations reduce to tautologies due to the Bianchi identities [51], which are identities involving the covariant derivatives of the Riemann tensor. More precisely, the Bianchi identities impose the following condition on the Einstein tensor

$$\nabla^{\mu} G_{\mu\nu} = 0.$$

It may be noted that by conservation of energy-momentum the stress-energy tensor is divergence free, i.e.,

$$\nabla^{\mu} T_{\mu\nu} = 0.$$

It is clear from the above discussion that there are only six independent equations in Einstein's field equations (5.5) where as the number of degrees of freedom are ten (the components of $g_{\mu\nu}$). Thus, the equations are inherently underdetermined. This indeterminacy is the gauge freedom of GR.

The *principle of covariance*, which is a fundamental postulate of GR extends the idea of Galilean invariance of Newtonian mechanics. According to this postulate, laws of physics must be the same in *all* reference frames. Mathematically, this statement may be expressed by requiring the equations to be invariant under *arbitrary* coordinate transformations. Thus, gauge freedom in GR stems from the reparametrization symmetry of the field equations (5.5). That is, the diffeomorphism group of coordinate transformations of the space-time forms a symmetry group of Einsteins equations.

Various gauge choices have been proposed in GR [56, 34, 58], the most popular being the *harmonic gauge* [58]. In this choice, the above six independent field equations are supplemented by the following four conditions on the coordinates x^μ,

$$\nabla_\alpha \nabla^\alpha x^\mu = 0, \quad \mu \in \{0, 1, 2, 3\}.$$

It is worth pointing out that the term *harmonic* is misleading. The preceding system of equations are not Laplace equations, since the underlying manifold is *pseudo*-Riemannian with a signature $(-, +, +, +)$. These equations are in fact wave equations on the coordinates.

5.3 Central Idea Behind Gauge Fixing

In this section, the essential idea behind gauge fixing is explained. For notational convenience, we shall restrict ourselves to the lipid membrane problem. The idea, however, is general and works for any problem with a gauge symmetry. Recall that the equilibrium equations for the membrane written abstractly as follows

$$\mathcal{F}(\mathbf{f}(\mathbf{X}), \phi(\mathbf{X})) = \mathbf{0}. \tag{5.8}$$

The reparametrization invariance of the system implies that if $(\mathbf{f}^*(\mathbf{X}), \phi^*(\mathbf{X}))$

is a solution, then so is $(f^* \circ h(\mathbf{X}), \phi^* \circ h(\mathbf{X}))$, for any diffeomorphism $h : S^2 \to S^2$. Solutions exist in an equivalence class.

To be able to explicitly solve for a solution, it is sufficient to pick any one solution from this equivalence class. The procedure to accomplish this is called *gauge fixing*. In this procedure, we replace the previous equation, (5.8), with the following system,

$$\mathcal{F}(\mathbf{f}(\mathbf{X}), \phi(\mathbf{X})) = \mathbf{0}, \tag{5.9}$$

$$\mathcal{G}(\mathbf{f}(\mathbf{X}), \phi(\mathbf{X})) = \mathbf{0}, \tag{5.10}$$

where $\mathcal{G}$ is suitably chosen such that the combined system has a unique solution, $(\hat{\mathbf{f}}(\mathbf{X}), \hat{\phi}(\mathbf{X}))$, in the equivalence class. It is clear that this solution will satisfy (5.8). By this prescription, the equation $\mathcal{G} = 0$ breaks the gauge symmetry completely and we have picked a representative solution from the equivalence class.

In the next few sections, we shall describe how to choose the right $\mathcal{G}$ for the lipid membrane.

5.4 Generalizing the Idea of Harmonic Functions

In section (5.2.2), we saw that a popular gauge fixing equation that is employed in GR is the harmonic condition on the coordinates. Since coordinate diffeomorphisms form a symmetry group of both GR and the lipid membrane equations, it may naively be assumed that the harmonic coordinate condition could be applied for lipid membranes, as well. However, the problem we run into is clear - the only harmonic functions on compact manifolds are constant functions (cf. corollary 4), which cannot be coordinate diffeomorphisms. The problem with this previous strategy is that while in GR the coordinates are $\mathbb{R}^4$ valued functions (with a Minkowiskiian metric), in the lipid membrane problem, the coordinates are S^2 valued functions. Therefore, we must look for a suitable generalization of harmonic

functions that take value in S^2. Fortunately, such a generalization of harmonic functions, called *harmonic map* has already been a subject of immense research [13, 14]. In the following section, we define the *harmonic energy* between manifolds as a generalization of the Dirichlet energy and present the *harmonic map equation* as the Euler-Lagrange equation of the corresponding harmonic energy. Details of the derivations can be found in [40], [42].

5.4.1 Harmonic Energy

Let (M, g) and (N, γ) be two Riemannian manifolds of dimensions m and n, and metric tensors $g_{\alpha\beta}$ and γ_{ij}, respectively. For any C^1 map $f : M \to N$ we define the *harmonic energy*,

$$e(f) = \int_M \frac{1}{2} g^{\alpha\beta} \gamma_{ij} \frac{\partial f^i(x)}{\partial x^\alpha} \frac{\partial f^j(x)}{\partial x^\beta} \sqrt{g} dx^1 \wedge dx^2 \cdots \wedge dx^m. \tag{5.11}$$

A *harmonic map* is defined to be the critical point of this functional.

Eels and LeMaire [13] give a physical interpretation behind the definition. According to them, if we imagine M to be made of, say, "rubber" and N of, say, "marble". The map f can be thought to constrain M to lie on N. The Euler-Lagrange equation of the harmonic energy represents "tension" in the "rubber" at each point. That is to say, f is a harmonic map if and only if f constrains M to lie on N in a position of elastic equilibrium.

5.4.2 Harmonic Map Equation

Harmonic maps are solutions to the Euler-Lagrage equation associated with harmonic energy, (5.11). By taking the variation of the functional (details can be found in [42]), we obtain the harmonic map equation,

$$\frac{1}{\sqrt{g}} \partial_\alpha \left(\sqrt{g} g^{\alpha\beta} \partial_\beta f^i \right) + g^{\alpha\beta} \Upsilon^i_{jk}(f(x)) \partial_\alpha f^j \partial_\beta f^k = 0, \tag{5.12}$$

where Υ^i_{jk} are the Christoffel symbols on N.

The previous equation can be abstractly written as follows,

$$\Delta_M f^i + \Upsilon^i_{jk} \langle \nabla f^j, \nabla f^k \rangle_M = 0, \tag{5.13}$$

where $\Delta_M(\cdot)$ is the Laplace-Beltrami on M and $\langle \cdot, \cdot \rangle_M$ is the inner product on M induced by its Riemannian metric.

In following special cases, the harmonic map equation reduces to familiar equations of mathematics.

1. If dim M = 1, the harmonic map equation reduces to the geodesic equation on N.
2. If $N = \mathbb{R}$, then it reduces to the familiar Laplace-Beltrami operator on M

It must be noted that the dependence of the Christoffel symbols, $\Upsilon^{\cdot}_{\cdot\cdot}$ on f makes the harmonic map equation a nonlinear PDE. General existence results to the harmonic map equation is therefore difficult. It has, nevertheless, been a subject of extensive research [13],[14], [43], [40], [55].

In this work, we concern ourselves only with results for 2-manifolds that are homeomorphic to S^2. That is, genus zero oriented surfaces.

An application of the harmonic map equation in this context is to conformally parametrize the 2-sphere. This idea has been explored and successfully applied to brain imaging studies [25], [24].

5.5 Existence of Harmonic Diffeomorphisms

Our motivation to study harmonic maps is to find a suitable candidate for the gauge-fixing equation. As discussed in section (5.3), the hope is to find a suitable coordinate system that breaks the gauge-symmetry. The harmonic map would be

a useful choice only if the resulting map provided a coordinate diffeomorphism. In this section, we shall see that there indeed does exist a harmonic diffeomorphism between a genus zero compact Riemannian (oriented) 2-manifold and S^2, thereby, substantiating our claim that the harmonic map equation (5.12) can be used as a gauge fixing equation for the lipid membrane problem.

We shall show the existence of harmonic diffeomorphisms in two steps. In the next section, we first show the existence of a conformal diffeomorphism between genus zero Riemannian surfaces and S^2. In the subsequent section we shall show that conformal diffeomorphisms between 2-manifolds are harmonic. The existence of harmonic diffeomorphisms follows from these two results.

5.5.1 Existence of Conformal Diffeomorphisms

Definition 9 (Conformal Mapping)**.** *A mapping $f : (M, g) \to (N, h)$ between Riemannian manifolds is said to be conformal if there exists a positive function $\lambda : M \to \mathbb{R}^+$ such that,*

$$h_{ij}(f(x))\frac{\partial f^i}{\partial x^\alpha}\frac{\partial f^j}{\partial x^\beta} = \lambda(x) g_{\alpha\beta}(x). \tag{5.14}$$

Remark 2.

1. *This means that the pull back of the metric on N is proportional (pointwise) to the metric on M.*
2. *Geometrically, this may be interpreted as the mapping f, preserves angles.*

If M is a genus zero compact oriented Riemannian manifold and N is S^2 with the usual metric, then the existence of a conformal mapping $f : M \to S^2$ is guaranteed by the following corollary to the Riemann-Roch theorem [40], [41].

Theorem 7 (Corollary to Riemann-Roch)**.** *Genus zero compact oriented Riemannian manifolds are conformally diffeomorphic to a two sphere.*

5.5.2 Conformal Diffeomorphisms are Harmonic

We now show that a conformal diffeomorphism between 2-manifolds is harmonic. Recall that $f : (M, g) \to (N, h)$ is conformal if the following condition is satisfied

$$h_{ij}(f(x))\partial_\alpha f^i \partial_\beta f^j = \lambda(x) g_{\alpha\beta}, \tag{5.15}$$

where $\lambda(x)$ is a positive function on M.

Differentiating the previous equation with respect to x^β, x^α and x^γ (and relabelling), we get

$$\partial_\beta \left(h_{kl}\partial_\alpha f^k \partial_\gamma f^l\right) = \lambda_\beta g_{\alpha\gamma} + \lambda \partial_\beta g_{\alpha\gamma}, \tag{5.16}$$

$$\partial_\alpha \left(h_{lj}\partial_\gamma f^l \partial_\beta f^j\right) = \lambda_\alpha g_{\gamma\beta} + \lambda \partial_\alpha g_{\gamma\beta}, \tag{5.17}$$

$$\partial_\gamma \left(h_{jk}\partial_\beta f^j \partial_\alpha f^k\right) = \lambda_\gamma g_{\beta\alpha} + \lambda \partial_\gamma g_{\beta\alpha}. \tag{5.18}$$

Combining the previous equations with appropriate signs and multiplying both sides with $g^{\alpha\beta}$.

$$g^{\alpha\beta}\left(\partial_j h_{kl} + \partial_k h_{lj} - \partial_l h_{jk}\right)\left(\partial_\alpha f^k \partial_\beta f^j \partial_\gamma f^l\right) + g^{\alpha\beta}\Big[h_{kl}\partial_\beta\left(\partial_\alpha f^k \partial_\gamma f^l\right) + h_{lj}\partial_\alpha\left(\partial_\gamma f^l \partial_\beta f^j\right) + h_{jk}\partial_\gamma\left(\partial_\alpha f^k \partial_\beta f^j\right)\Big] = 2\lambda g^{\alpha\beta} g_{\gamma\mu}\Gamma^\mu_{\alpha\beta} + (2 - \delta^\alpha_\alpha)\partial_\gamma\lambda.$$

Note that for a 2-manifold, $\delta^\alpha_\alpha = 2$. Therefore, the last term in the previous expression vanishes. We now replace the partials of the metric $h_{..}$ in terms of its Christoffel symbols $\Upsilon^{\cdot}_{\cdot\cdot}$. We then expand the terms in the (square) brackets. After a bit of relabeling, the previous equation reduces to

$$2g^{\alpha\beta}h_{il}\Upsilon^i_{jk}\left(\partial_\alpha f^k \partial_\beta f^j \partial_\gamma f^l\right) + 2g^{\alpha\beta}h_{il}\partial^2_{\alpha\beta} f^i \partial_\gamma f^l = 2\lambda g^{\alpha\beta} g_{\gamma\mu}\Gamma^\mu_{\alpha\beta}.$$

We now use equation (5.15) to rewrite $\lambda g_{\gamma\mu}$ as $h_{il}\partial_\gamma f^l \partial_\mu f^i$. With this, λ can be eliminated and we have,

$$2g^{\alpha\beta}h_{il}\Upsilon^i_{jk}\left(\partial_\alpha f^k \partial_\beta f^j \partial_\gamma f^l\right) + 2g^{\alpha\beta}h_{il}\partial^2_{\alpha\beta} f^i \partial_\gamma f^l = 2g^{\alpha\beta}\Gamma^\mu_{\alpha\beta}h_{il}\partial_\gamma f^l \partial_\mu f^i.$$

We finally note that $g^{\alpha\beta}\Gamma^{\mu}_{\alpha\beta} = -\frac{1}{\sqrt{g}}\partial_\alpha(\sqrt{g}g^{\mu\alpha})$. Thus, we have,

$$2g^{\alpha\beta}h_{il}\Upsilon^i_{jk}\left(\partial_\alpha f^k\partial_\beta f^j\partial_\gamma f^l\right) + 2g^{\alpha\beta}h_{il}\partial^2_{\alpha\beta}f^i\partial_\gamma f^l + 2\frac{1}{\sqrt{g}}\partial_\alpha(\sqrt{g}g^{\mu\alpha})h_{il}\partial_\gamma f^l\partial_\mu f^i = 0.$$

That is,

$$\Big[\frac{1}{\sqrt{g}}\partial_\alpha\left(\sqrt{g}g^{\alpha\beta}\partial_\beta f^i\right) + g^{\alpha\beta}\Upsilon^i_{jk}\partial_\alpha f^j\partial_\beta f^k\Big]h_{il}\partial_\gamma f^l = 0. \tag{5.19}$$

Since f is a diffeomorphism, its jacobian is invertible. This lets us conclude that,

$$\Big[\frac{1}{\sqrt{g}}\partial_\alpha\left(\sqrt{g}g^{\alpha\beta}\partial_\beta f^i\right) + g^{\alpha\beta}\Upsilon^i_{jk}\partial_\alpha f^j\partial_\beta f^k\Big] = 0. \tag{5.20}$$

That is, f is a harmonic map.

5.6 Harmonic Gauge for Closed Lipid Membranes

It is clear from the previous discussion that there exists a harmonic diffeomorphism $f : \omega \to S^2$, provided, ω is a genus zero compact surface. We use the harmonic map equation to construct a gauge fixing condition for the closed lipid membrane problem. In what follows, $g_{\alpha\beta}$ represents the metric tensor of the lipid membrane surface ω and Υ is the Christoffel symbol of the two sphere S^2.

The harmonic map equation, as seen from equation (5.13), can be written independent of coordinates. Therefore, any suitable coordinate system can be used to write the harmonic map equation. We choose to rewrite the equation in terms of the harmonic coordinates. That is, we parametrize ω in terms of (f^1, f^2). Under this change of coordinates,

$$g^{\alpha\beta} = \tilde{g}^{\mu\nu}\frac{\partial x^\alpha}{\partial f^\mu}\frac{\partial x^\beta}{\partial f^\nu}.$$

The determinant of the metric tensor transforms as follows,

$$\sqrt{g} = \sqrt{\tilde{g}}\det\left(\frac{\partial f^\mu}{\partial x^\alpha}\right),$$

$$\frac{1}{\sqrt{g}} = \frac{1}{\sqrt{\tilde{g}}} \det\left(\frac{\partial x^\alpha}{\partial f^\mu}\right).$$

The harmonic map equation then can be written as,

$$\frac{1}{J_f\sqrt{\tilde{g}}}\frac{\partial f^\sigma}{\partial x^\alpha}\frac{\partial}{\partial f^\sigma}\left(\sqrt{\tilde{g}}J_f\tilde{g}^{\mu\nu}\frac{\partial x^\alpha}{\partial f^\mu}\frac{\partial x^\beta}{\partial f^\nu}\frac{\partial f^\tau}{\partial x^\beta}\right) + \tilde{g}^{\mu\nu}\frac{\partial x^\alpha}{\partial f^\mu}\frac{\partial x^\beta}{\partial f^\nu}\Upsilon^\tau_{\sigma\eta}\frac{\partial f^\sigma}{\partial x^\alpha}\frac{\partial f^\eta}{\partial x^\beta} = 0.$$

For convenience, we define the following jacobian tensor and its determinant

$$A^\alpha_\mu := \frac{\partial x^\alpha}{\partial f^\mu,} \tag{5.21}$$

$$A = \det\left(A^\alpha_\mu\right).$$

The inverse of the jacobian can be written as,

$$(A^{-1})^\mu_\alpha = \frac{\partial f^\mu}{\partial x^\alpha}.$$

The harmonic map equation can then be written as,

$$\frac{A}{\sqrt{\tilde{g}}}(A^{-1})^\sigma_\alpha\frac{\partial}{\partial f^\sigma}\left(\frac{\sqrt{\tilde{g}}}{A}\tilde{g}^{\mu\tau}A^\alpha_\mu\right) + \tilde{g}^{\mu\nu}\Upsilon^\tau_{\mu\nu} = 0.$$

Note that $A(A^{-1})^\sigma_\alpha$ is the cofactor matrix of the jacobian (defined in equation (5.21)) and therefore is divergence-free. With this observation, the previous equation simplifies to,

$$\frac{1}{\sqrt{\tilde{g}}}\frac{\partial}{\partial f^\sigma}\left(\frac{\sqrt{\tilde{g}}}{A}\tilde{g}^{\mu\tau}A^\alpha_\mu A(A^{-1})^\sigma_\alpha\right) + \tilde{g}^{\mu\nu}\Upsilon^\tau_{\mu\nu} = 0.$$

Cancelling terms, we have

$$\frac{1}{\sqrt{\tilde{g}}}\partial_\alpha\left(\sqrt{\tilde{g}}\tilde{g}^{\alpha\beta}\right) + \Upsilon^\beta_{\mu\nu}(f)\tilde{g}^{\mu\nu} = 0, \tag{5.22}$$

where all the partials are now taken with respect to f^μ.

That is, the previous equation (5.22), is the harmonic map equation when the surface ω is itself parametrized in terms of harmonic coordinates.

Let us choose $(\vartheta, \varphi) \in S^2$, the canonical spherical coordinates, to represent the harmonic coordinates that we wish to solve for. In these coordinates, the harmonic map equations can be written as follows,

$$\frac{1}{\sqrt{g}}\partial_\alpha\Big(\sqrt{g}g^{\alpha\vartheta}\Big) - \sin(\vartheta)\cos(\vartheta)g^{\varphi\varphi} = 0, \tag{5.23a}$$

$$\frac{1}{\sqrt{g}}\partial_\alpha\Big(\sqrt{g}g^{\alpha\varphi}\Big) + \cot(\vartheta)g^{\vartheta\varphi} = 0. \tag{5.23b}$$

The terms $-\sin(\vartheta)\cos(\vartheta)$ and $\cot(\vartheta)$ in the previous equations are the appropriate Christoffel symbols on S^2 in spherical coordinates.

5.6.1 Möbius Transformations

Let us note that harmonic map equation (5.12) when used as a gauge-fixing equation is at best an incomplete gauge. This is because if $f : M \to S^2$ is a harmonic diffeomorphism then so is $f \circ \mu : M \to S^2$, where $\mu : S^2 \to S^2$ is any conformal/harmonic diffeomorphism of S^2. It is therefore not possible to break the gauge symmetry completely by just using the harmonic map equation. Let us note that the set of all conformal (and hence harmonic) diffeomorphisms of S^2 forms a six dimensional Lie group called the Möbius group. Therefore, using the harmonic equation we have broken the gauge symmetry from an infinite dimensional diffeomorphism group of S^2 to a six dimensional Möbius group.

The relation between Möbius group as the conformal diffeomorphism group of S^2 and the group of linear fractional transformations of the complex plane becomes apparent if the sphere is viewed as a one point compactification of the complex plane. Furthermore, the Möbius transformations may be visualized as the rigid motions of this projective sphere [3]. By taking this point of view, the freedom of the Möbius group may be constrained by fixing the rigid motions of the sphere.

Such an approach has been implemented in the context of brain imaging in [24]. For our purpose here, in the case of axisymmetric solutions, the following constraint may be added to the gauge-fixing equation to fix the gauge completely.

$$\int_{S^2} \cos(\vartheta)\sqrt{g}\, d\vartheta = 0. \tag{5.24}$$

CHAPTER 6

COMPUTATIONS - EQUILIBRIA

6.1 Introduction

The previous chapters were mainly concerned with theoretical aspects of the problem. We have formulated the governing equilibrium equations, presented the second variation required to compute stability of equilibria, established local existence of symmetry-breaking branches and proposed a gauge fixing procedure for the problem. In this chapter, we consider the computational aspects of the problem.

The nonlinearity of the problem and the dependence on various parameters makes the behavior of equilibria extremely diverse. For truly understanding the system, we must resort to a systematic approach to computation for analyzing the problem. Numerical continuation, also called path following, is one such method by which the parameter space can be explored by plotting bifurcation diagrams. In the next few sections we shall briefly summarize the basics of path following. More details can be found in [1, 45, 66]. We then use these ideas to numerically solve the equilibrium equations (2.30) supplemented with the gauge fixing conditions (5.23), *viz.,* the gauge fixed formulation.

Any numerical approach to solving partial differential equations involves projecting the equations onto a finite dimensional function space. We employ a Galerkin projection to discretize the equilibrium equations and obtain the weak form. In this work, we restrict ourselves only to axisymmetric solutions. Accordingly, we represent the the position vector $\mathbf{f}(\mathbf{X})$ of the surface ω in terms of its radial and tangential components. The surface is discretized into elements and we associate each element with nodal variables which will be the unknowns of the discretized system. Hermite cubics will be used to interpolate the nodal variables

over the element.

This chapter is concerned only with the computational aspects of equilibria. Determining stability by discretizing the hessian will be discussed in the next chapter.

6.2 Numerical Path Following

In this section, we shall briefly summarize the basic ideas of path following. More details can be found in [1],[45].

Let us write the discretized equations that we wish to solve, abstractly, as follows

$$\mathbf{F}(\mathbf{y}, \lambda) = \mathbf{0}, \tag{6.1}$$

where $\mathbf{F} : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^n$ is the unknown vector of interest and λ is a parameter of the system.

In numerical continuation, we trace the solutions $\mathbf{y}$ of the previous equation (6.1) as a function of the parameter λ. This plot is usually called the *bifurcation diagram*. A schematic bifurcation diagram is shown in figure (6.1). While performing continuation, we typically start with a solution that is known *a priori*, $(\mathbf{y}_o, \lambda_o)$ and trace the solutions in its vicinity as we vary λ. This curve is usually called a *primary solution branch*. It may also be referred to as *trivial solution branch* in the case when the whole branch may be known *a priori*. In this case, without loss of generality, we may normalize the primary solution to $(\mathbf{0}, \lambda_o)$.

A typical bifurcation diagram has points where branches lose uniqueness - either due to 1) bending of the branch onto itself, called the *limit point or turning point* or 2) due to multiple branches intersecting each other, called *branch point or bifurcation point*. A bifurcation point can further be classified as *simple* or *multiple*. A solution branch that intersects a primary bifurcation path is referred

to as *secondary bifurcation path.* A schematic showing these possibilities has been provided in figure (6.1).

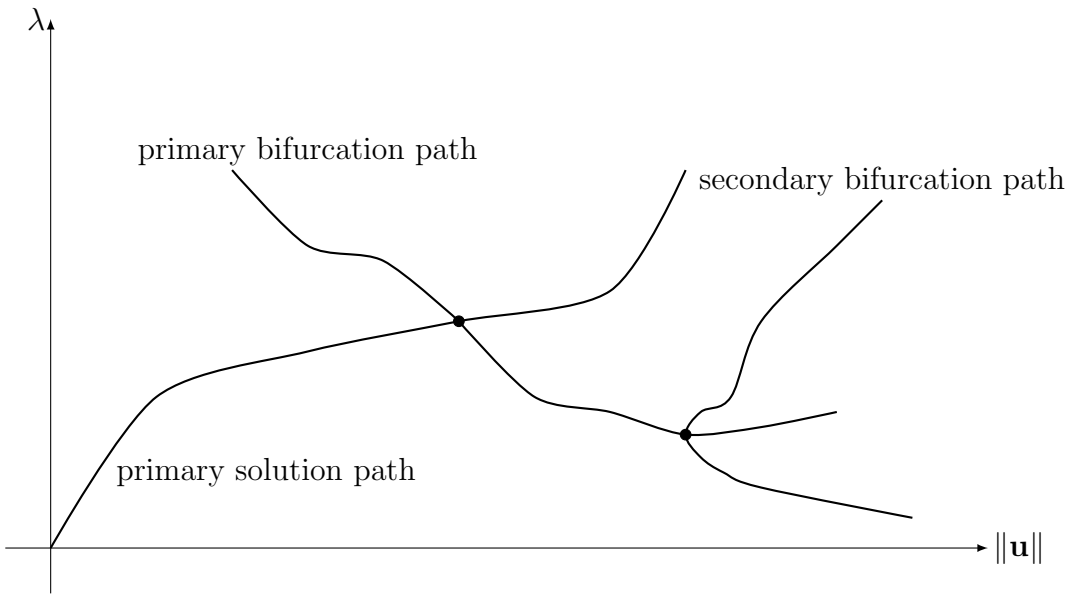


Figure 6.1: Schematic Bifurcation Diagram

Let us introduce the following definitions,

Definition 10 (Branch Point)**.** *We say that a point* $(\mathbf{y}_o, \lambda_o)$ *is a* branch point *to a path of solutions if every sufficiently small neighborhood of* $(\mathbf{y}_o, \lambda_o)$ *contains solutions* $(\mathbf{y}, \lambda)$ *not included in the former path.*

Definition 11 (Regular Point)**.** *A solution,* $(\mathbf{y}_o, \lambda_o)$ *to equation (6.1) is called a* regular point *if* $\mathbf{F}_{\mathbf{y}}(\mathbf{y}_o, \lambda_o)$ *is invertible.*

Definition 12 (Limit Point)**.** *A solution* $(\mathbf{y}_o, \lambda_o)$ *to equation (6.1) is called a* limit point *if* $D_{\mathbf{y}}\mathbf{F}(\mathbf{y}_o, \lambda_o)$ *is not invertible and*

$$D_\lambda \mathbf{F}(\mathbf{y}_o, \lambda_o) \notin \ Range\Big(D_{\mathbf{y}}\mathbf{F}(\mathbf{y}_o, \lambda_o)\Big). \tag{6.2}$$

For notational convenience, we make the following definition,

$$\mathbf{K}(\mathbf{y}_o, \lambda_o) := \mathbf{F}_{\mathbf{y}}(\mathbf{y}_o, \lambda_o).$$

It can be shown [26] that the local form of the solution branch passing through a simple limit point $(\mathbf{y}_o, \lambda_o)$ is given by

$$\mathbf{y}(s) = \mathbf{y}_o + s\boldsymbol{\phi}_o + o(s), \tag{6.3a}$$

$$\lambda(s) = \lambda_o + o(s), \tag{6.3b}$$

where s in the previous equation is a suitable parametrization of the path and $\boldsymbol{\phi}_o$ is a null vector of $\mathbf{K}_o$.

6.2.1 Euler Continuation

Since we are interested in the solutions $\mathbf{y}$ of (6.1) as a function of λ, we may (naively) parametrize $\mathbf{y}$ in terms of λ, that is, $\mathbf{y}(\lambda)$. If $\mathbf{F}$ is assumed to be sufficiently smooth, we may differentiate equation (6.1) and write the resultant equation as follows,

$$\mathbf{F}_{\mathbf{y}}(\mathbf{y}(\lambda), \lambda)\dot{\mathbf{y}}(\lambda) = -\mathbf{F}_{\lambda}(\mathbf{y}(\lambda), \lambda), \tag{6.4}$$

where $\dot{\mathbf{y}}(\lambda) = \frac{d\mathbf{y}}{d\lambda}(\lambda)$.

If $\mathbf{F}_{\mathbf{y}}$ is invertible at some point $(\mathbf{y}_o, \lambda_o)$, then we can invert the previous equation (6.4) and using the Implicit Function Theorem, we have a unique solution branch in the neighborhood of $(\mathbf{y}_o, \lambda_o)$. Computing this branch is called numerical path-following. The process can be broadly divided into the following two steps:

1. **Predictor Step:** In this step, we generate a guess for a new solution of the equation (6.1) close to a known solution, $(\mathbf{y}_o, \lambda_o)$. The simplest of such schemes, called the Euler-method, would be

$$(\mathbf{y}_1, \lambda_1) = (\mathbf{y}_o, \lambda_o + \Delta\lambda). \tag{6.5}$$

2. **Corrector Step:** In this step, we refine the guess, (6.5), from the predictor step using an iterative procedure to converge to a solution $(\mathbf{y}_*, \lambda+\Delta\lambda)$. There

are a variety of such iterative procedures available, eg. Newton's method, Secant Method, Broyden method, etc. [1], [45].

Algorithm: Euler Continuation

Define λ as an arc-length parameter. Assuming a solution point $(\mathbf{y}_o, \lambda_o)$ is known, a nearby solution, $\lambda^* = \lambda_o + \Delta\lambda$, is sought, where $\Delta\lambda$ is some sufficiently small increment of λ. A new solution point,

$$(\mathbf{y}^*, \lambda^*) = (\mathbf{y}_o + \Delta\mathbf{y}, \lambda^*),$$

is defined by finding $\Delta\mathbf{y}$ that satisfies,

$$\mathbf{F}(\mathbf{y}_o + \Delta\mathbf{y}, \lambda^*) = \mathbf{0}.$$

1. (Prediction Step) Define an initial approximate guess for $\mathbf{y}^* \approx \mathbf{y}_1 = \mathbf{y}_o + \Delta Y_o$ where $\Delta\mathbf{y}_o$ is the solution to

$$\mathbf{K}_o \Delta\mathbf{y}_o = -\Delta\lambda \mathbf{F}_\lambda. \tag{6.6}$$

2. (Corrector Step) We now perform a Newton iteration to refine the initial guess $\mathbf{y}_1$, by iterative updates $\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta Y_n$, where ΔY_n is obtained by solving,

$$\mathbf{K}(\mathbf{y}_n, \lambda^*)\Delta\mathbf{y}_n = -\mathbf{F}(\mathbf{y}_n, \lambda^*),$$

   until a convergence criterion $||\mathbf{F}(\mathbf{y}_{n+1}, \lambda^*)|| < \tau$ is met, where τ is a suitably chosen tolerance.

3. The previous steps are repeated to search for the next point using the previously computed $(\mathbf{y}^*, \lambda^*)$ as the starting point.

It is possible, with sufficient smoothness of the branches [45] to be able to continue past singular points such as bifurcation points. However, a major drawback of

Euler continuation is that it breaks down at limit points, where $\mathbf{F_y}$ is not invertible and $\mathbf{F}_\lambda(\mathbf{y}_o, \lambda_o) \notin \ Range\Big(\mathbf{F_y}(\mathbf{y}_o, \lambda_o)\Big)$. The way to fix this is to modify the above procedure by introducing a parametrization for the path. This method, called arc-length continuation, will be presented in the next section.

6.2.2 Arc-Length Continuation

To overcome the drawback of Euler's method discussed in the previous section, let us parametrize the solution as $(\mathbf{y}(s), \lambda(s))$, where s is a conveniently chosen parameter, usually arc-length or some measure of arc-length. In arc-length continuation, we append a scalar equation, $N(\mathbf{y}(s), \lambda(s), s) = 0$, for a suitable choice of N. We thus the have the following system to solve,

$$\begin{aligned} \mathbf{F}(\mathbf{y}(s), \lambda(s)) &= \mathbf{0}, \\ N(\mathbf{y}(s), \lambda(s), s) &= 0. \end{aligned} \tag{6.7}$$

For sufficiently smooth $\mathbf{F}$ and N, differentiating the previous system with respect to s and rearranging, we have

$$\begin{pmatrix} \mathbf{F_y} & \mathbf{F}_\lambda \\ \frac{\partial N}{\partial \mathbf{y}} & \frac{\partial N}{\partial \lambda} \end{pmatrix} \begin{pmatrix} \dot{\mathbf{y}}(s) \\ \dot{\lambda}(s) \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ -\frac{\partial N}{\partial s} \end{pmatrix}. \tag{6.8}$$

There are a number of suggested choices for N [45],[44]. The most popular is the so called *pseudo arc-length method*, in which,

$$N(\mathbf{y}, \lambda, s) = (\mathbf{y} - \mathbf{y}_o) \cdot \dot{\mathbf{y}}_o + (\lambda - \lambda_o)\dot{\lambda}_o = (s - s_o). \tag{6.9}$$

It can be shown that, [45], at a limit point the matrix $\begin{pmatrix} \mathbf{F_y} & \mathbf{F}_\lambda \\ \frac{\partial N}{\partial \mathbf{y}} & \frac{\partial N}{\partial \lambda} \end{pmatrix}$ is invertible, even though $\mathbf{F_y}$ is itself not invertible. It is, therefore, possible to continue past limit point without any difficulty.

We now summarize the algorithm for pseudo-arclength method as found in [66].

Algorithm: Pseudo-Arc Length Continuation

Assuming that a solution point $(\mathbf{y}_o(s_o), \lambda_o(s_o), s_o)$ is known, a nearby solution located at $s^* = s_o + \Delta s$ is sought.

1. Define an initial guess for $(\mathbf{y}^*, \lambda^*)$ as,

$$\mathbf{y}_1 = \mathbf{y}_o + \Delta s \dot{\mathbf{y}}_o,$$

$$\lambda_1 = \lambda_o + \Delta s \dot{\lambda}_0.$$

   Near a limit point, differentiating (6.3), we see that $\dot{\mathbf{y}}_o$ and $\dot{\lambda}_o$ can be taken to be

$$\dot{Y}_o = \boldsymbol{\phi}_o, \quad \dot{\lambda}_o = 0,$$

   where $\boldsymbol{\phi}_o$ is the null vector of $\boldsymbol{K}_o$.

   If $(\mathbf{y}_o, \lambda_o)$ is not near limit point, then $\dot{\mathbf{y}}_o$ and $\dot{\lambda}_o$ are chosen to be

$$\dot{\mathbf{y}}_o = -\frac{\mathbf{w}}{(\mathbf{w} \cdot \mathbf{w} + 1)^{(1/2)}}, \ \dot{\lambda}_o = \frac{1}{(\mathbf{w} \cdot \mathbf{w} + 1)^{(1/2)}},$$

   where $\mathbf{w}$ is the solution to

$$\mathbf{K}_o \mathbf{w}_o = \mathbf{F}_\lambda^o.$$

2. Refine the initial guess $(\mathbf{y}_1, \lambda_1)$ by the following updates,

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta \mathbf{y}_n,$$

$$\lambda_{n+1} = \lambda_n + \Delta \lambda_n,$$

   where $\Delta \mathbf{y}_n$ and $\Delta \lambda_n$ are given by

$$\Delta \lambda_n = \frac{N_n - \dot{\mathbf{y}}_o \cdot \mathbf{p}_n}{\dot{\mathbf{y}}_o \cdot \mathbf{q}_n - \dot{\lambda}_o},$$

$$\Delta \mathbf{y}_n = -\mathbf{p}_n - \mathbf{q}_n \Delta \lambda_n,$$

where,

$$N_n := \dot{\mathbf{y}}_o \cdot (\mathbf{y}_n - Y_o) + \dot{\lambda}_o(\lambda_n - \lambda_o) - \Delta s,$$

and $\mathbf{p}_n$ and $\mathbf{q}_n$ are solutions to

$$\mathbf{K}(\mathbf{y}_n, \lambda_n)\mathbf{p}_n = \mathbf{F}(\mathbf{y}_n, \lambda_n),$$

$$\mathbf{K}(\mathbf{y}_n, \lambda_n)\mathbf{q}_n = \mathbf{F}_\lambda(\mathbf{y}_n, \lambda_n).$$

Continue this step until convergence criterion

$$||\Big(\mathbf{F}(\mathbf{y}_{n+1}(s^*), \lambda(s^*), N(\mathbf{y}_{n+1}(s^*), \lambda^*(s^*), s^*))\Big)|| < \tau$$

is met.

3. The previous steps are repeated to search for the next point using the previously computed $(\mathbf{y}^*, \lambda^*, s^*)$ as the starting point.

We use this algorithm to compute our solution branches presented in chapter (8).

6.2.3 Bifurcations and Branch Switching

Branch switching in the case of a *simple bifurcation point* (all the cases treated in this dissertation) is relatively straightforward. It is done by choosing the following as the guess for the starting point in predictor step of the new branch,

$$\mathbf{y}_1 = \mathbf{y}_o + \alpha\boldsymbol{\phi},$$

where α is suitably chosen to achieve convergence of the newton scheme and the vector $\boldsymbol{\phi}$ is the null vector of the Hessian K_o.

6.3 Finite Element Formulation: Axisymmetric Problem

In this section, we present the finite element formulation to discretize the gauge fixed system of Euler-Lagrange equations . Instead of discretizing the energy functional (2.6a), using a Ritz approach, we apply a Galerkin projection to the Euler-Lagrange system, (2.30), supplemented with the gauge fixing harmonic map equation, (5.23). Later in this section, we specialize to the axisymmetry case and use Hermite cubic interpolation to discretize the displacement and the concentration fields.

6.3.1 Weak Form

Let $\boldsymbol{e}_r$, $\boldsymbol{e}_\vartheta$, $\boldsymbol{e}_\varphi$ be the normalized spherical basis vectors as shown in figure (6.2). Explicitly, these vectors can be written in terms of the standard cartesian basis $(\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k})$ as follows,

$$\boldsymbol{e}_r = \sin\vartheta\cos\varphi\boldsymbol{i} + \sin\vartheta\sin\varphi\boldsymbol{j} + \cos\vartheta\boldsymbol{k}, \tag{6.10a}$$

$$\boldsymbol{e}_\vartheta = \cos\vartheta\cos\varphi\boldsymbol{i} + \cos\vartheta\sin\varphi\boldsymbol{j} - \sin\vartheta\boldsymbol{k}, \tag{6.10b}$$

$$\boldsymbol{e}_\varphi = -\sin\varphi\boldsymbol{i} + \cos\varphi\boldsymbol{j}. \tag{6.10c}$$

To obtain the weak form via Galerkin projection, we multiply the Euler-Lagrange equations, (2.30), by test functions w and ψ and integrate by parts,

$$\int_\omega -c_g'(\phi)\tilde{b}^{\alpha\beta}w_\alpha\phi_\beta + c(\phi)H\Delta w + \Big\{2cH(H^2-K) + \epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta - 2\tilde{\gamma}H - p\Big\}w\ da = 0, \tag{6.11a}$$

$$\int_\omega \epsilon\nabla\psi\cdot\nabla\phi + \Big[W' + \lambda + c'H^2 + c_g'K\Big]\psi\ da = 0. \tag{6.11b}$$

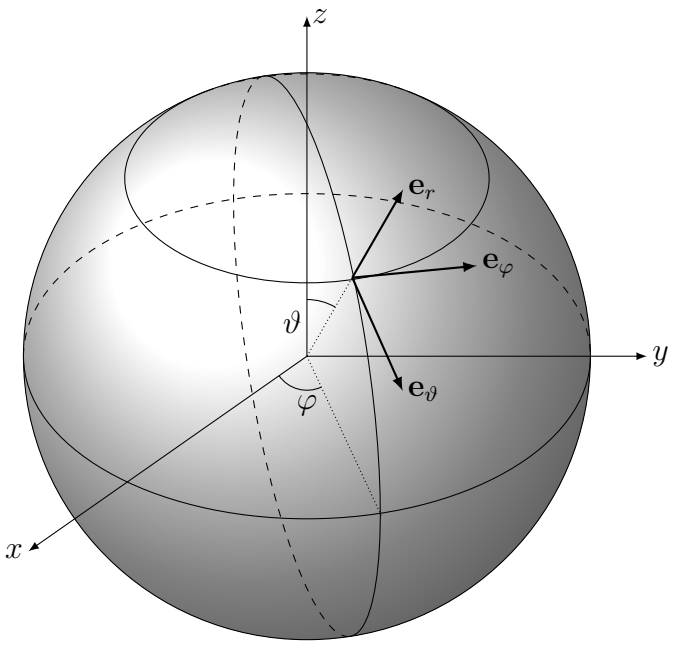


Figure 6.2: Coordinate System

Weak form for the gauge equations is obtained by multiplying the equations (5.23), by a test functions $v_\alpha,\ \alpha \in \{1, 2\}$,

$$\int_\omega \Big\{ \frac{1}{\sqrt{g}} \partial_\alpha \Big(\sqrt{g} g^{\alpha\beta} \Big) + \Upsilon^\beta_{\mu\nu} g^{\mu\nu} \Big\} v_\beta \, dA = 0, \tag{6.11c}$$

where Υ is the Christoffel symbol on the two sphere.

The associated constraints are,

$$\begin{aligned} \int_\omega da &= 4\pi, \\ \int_\omega (\phi - \mu) \, da &= 0. \end{aligned} \tag{6.11d}$$

6.3.2 Axisymmetric Formulation

In this work, we only consider axisymmetric equilibria. Two independent variables are required to describe a two dimensional axisymmetric surface. We choose them

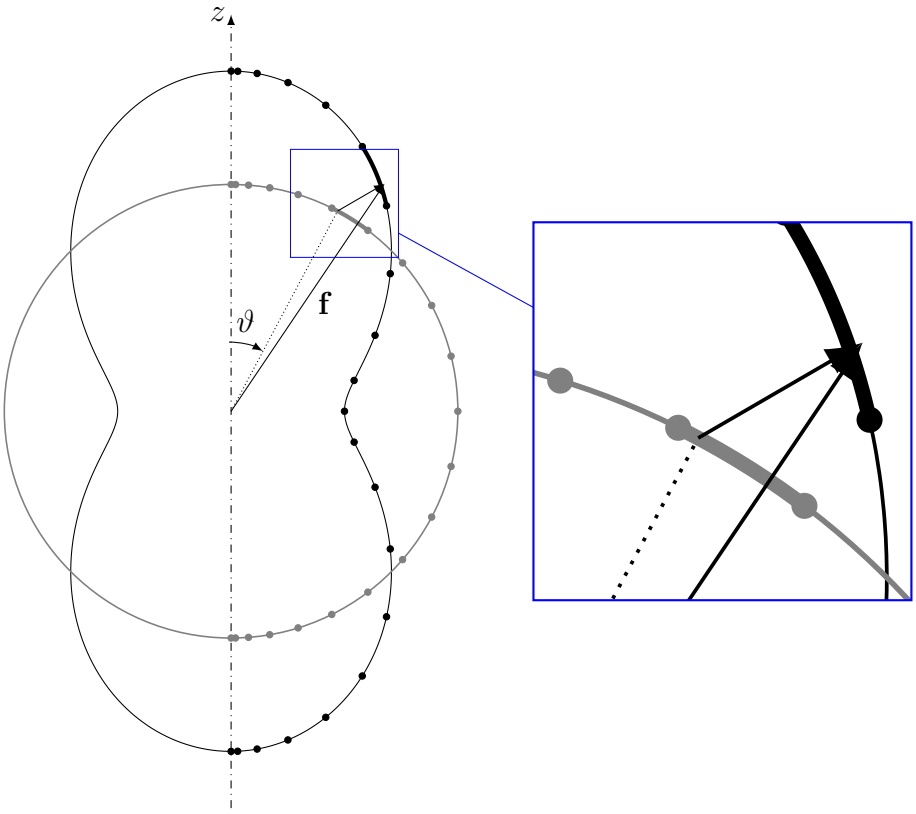


Figure 6.3: Discretized Schematic

to be the radial(u) and tangential(v) components of the position $\mathbf{f}$ from a spherical state. That is,

$$\mathbf{f}(\vartheta,\varphi) = u(\vartheta)\boldsymbol{e}_r(\vartheta,\varphi) + v(\vartheta)\boldsymbol{e}_\vartheta(\vartheta,\varphi). \tag{6.12}$$

The dependence of u and v solely on ϑ is due to axisymmetry. Similarly, the concentration field is only a function of ϑ.

Axisymmetry necessitates that the following boundary conditions must be imposed,

$$u'(0) = u'(\pi) = 0,\ v(0) = v(\pi) = 0,\ \phi'(0) = \phi'(\pi) = 0. \tag{6.13}$$

By integrating out the azimulthal angle φ, the weak form (6.11), is specialized to,

$$\int_0^\pi \Big[- c_g'(\phi)\tilde{b}^{\vartheta\vartheta} w_\vartheta \phi_\vartheta + c(\phi) H\,(\Delta w) + \Big\{ 2cH(H^2-K) + \epsilon b^{\vartheta\vartheta}\phi_\vartheta\phi_\vartheta - 2\tilde{\gamma}H - p \Big\} w \Big] + \lambda_z \Big(\cos\vartheta(n_r - 2Hu) - \sin\vartheta(n_\vartheta - 2Hv) \Big) \sqrt{g}\, d\vartheta = 0, \tag{6.14a}$$

$$\int_0^\pi \Big[\epsilon g^{\vartheta\vartheta}\phi_\vartheta\psi_\vartheta + \Big(W' + \lambda + c' H^2 + c_g' K \Big)\psi \Big] \sqrt{g}\, d\vartheta = 0, \tag{6.14b}$$

$$\int_0^\pi \Big[\frac{1}{\sqrt{g}} \partial_\vartheta \Big(\sqrt{g} g^{\vartheta\vartheta} \Big) - \sin(\vartheta)\cos(\vartheta) g^{\varphi\varphi} + \lambda_g \sin\vartheta \Big] \sqrt{g}\, d\vartheta = 0, \tag{6.14c}$$

where we have used the fact that for axisymmetric solutions, $g^{\vartheta\varphi} = 0$.

In the above equations, n_r and n_ϑ are the components of the normal in the $\boldsymbol{e}_r$ and $\boldsymbol{e}_\vartheta$ direction. The Lagrange multiplier λ_z enforces the constraint that the z-component of the center of mass is fixed, *i.e.,*

$$\int_0^\pi (u\boldsymbol{e}_r + v\boldsymbol{e}_\vartheta) \cdot \boldsymbol{k}\ \sqrt{g} d\vartheta = 0. \tag{6.14d}$$

The Lagrange multiplier λ_g enforces the following constraint for Möbius transformations,

$$\int_0^\pi \cos\vartheta\ \sqrt{g} d\vartheta = 0. \tag{6.14e}$$

The incompressibility and concentration constraints discussed earlier can be written as follows,

$$\int_0^\pi \sqrt{g}\, d\vartheta = 4\pi, \tag{6.14f}$$

$$\int_0^\pi (\phi - \mu)\sqrt{g}\, d\vartheta = 0. \tag{6.14g}$$

In the above equations H, K, $b^{\vartheta\vartheta}$, etc. can be computed in terms of the position vector, $\mathbf{f}$ and its derivatives.

6.3.3 Discretization

We use Hermite elements to approximate the position and the concentration variable. The interval $[0, \pi]$ is divided into *elements* $\Omega_e := [\vartheta^{e-1}, \vartheta^e]$, as shown in the figure (6.4),

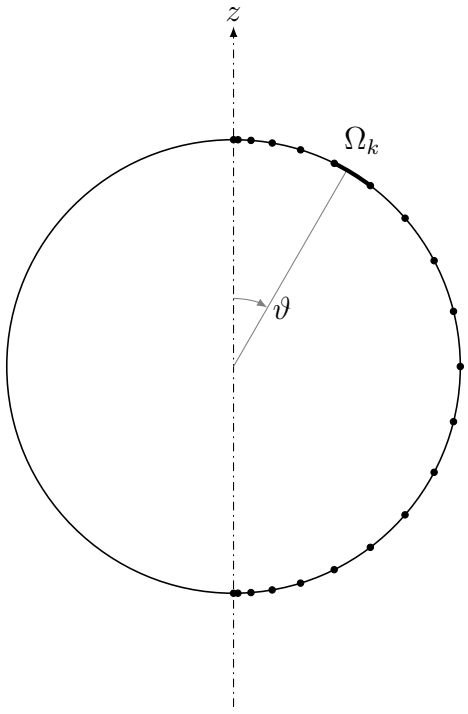
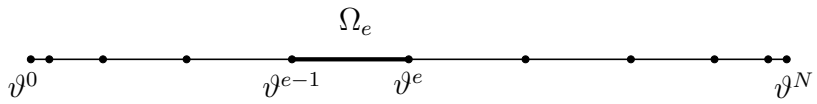


Figure 6.4: Discretization

Let N represent the total number of elements. We have the following partition for the interval,

$$[0, \pi] = \bigcup_{e=1}^{N} \Omega_e, \tag{6.15}$$

where $\vartheta^0 = 0$ and $\vartheta^N = \pi$.



For discretizing, every element Ω_e, is associated with a set of degrees of freedom called *nodal variables*. For Hermite cubics, there are two degrees of freedom per node - the value of the function at the node and its slope at the node. Thus, for node e we have the following unknowns,

$$\mathbf{y}_e = \Big(u_e, u'_e, v_e, v'_e, \phi_e, \phi'_e\Big)^T_{1\times 6}. \tag{6.16}$$

The boundary nodes, however, must be treated separately to incorporate the boundary conditions. For the left boundary ($\vartheta = 0$), we require the variables,

$$\mathbf{y}_0 = \Big(u_0, v'_0, \phi_0\Big)^T_{1\times 3}, \tag{6.17a}$$

and for the right boundary ($\vartheta = \pi$), we require,

$$\mathbf{y}_N = \Big(u_N, v'_N, \phi_N\Big)^T_{1\times 3}. \tag{6.17b}$$

We define the following vector for the Lagrange multipliers of the problem,

$$\boldsymbol{\ell} = \Big(\lambda, \gamma, \lambda_z, \lambda_g\Big)^T. \tag{6.17c}$$

For all elements Ω_e, except the first ($e = 1$) and the last ($e = N$), the variables u, v, ϕ are interpolated on the element (for which $\vartheta \in [\vartheta^{e-1}, \vartheta^e]$) using Hermite cubics as follows,

$$u(\vartheta) = u_{e-1}N_0^e(\vartheta) + u'_{e-1}N_1^e(\vartheta) + u_e N_2^e(\vartheta) + u'_e N_3^e(\vartheta), \tag{6.18a}$$

$$v(\vartheta) = v_{e-1}N_0^e(\vartheta) + v'_{e-1}N_1^e(\vartheta) + v_eN_2^e(\vartheta) + v'_eN_3^e(\vartheta), \tag{6.18b}$$

$$\phi(\vartheta) = \phi_{e-1}N_0^e(\vartheta) + \phi'_{e-1}N_1^e(\vartheta) + \phi_eN_2^e(\vartheta) + \phi'_eN_3^e(\vartheta), \tag{6.18c}$$

where the Hermite cubics on the element $\Omega_e = [\vartheta^{e-1}, \vartheta^e]$ are defined by the following polynomials,

$$N_0^e(\vartheta) := (2t_e^3 - 3t_e^2 + 1), \tag{6.19a}$$

$$N_1^e(\vartheta) := (t_e^3 - 2t_e^2 + t_e)h_e, \tag{6.19b}$$

$$N_2^e(\vartheta) := (-2t_e^3 + 3t_e^2), \tag{6.19c}$$

$$N_3^e(\vartheta) := (t_e^3 - t_e^2)h_e, \tag{6.19d}$$

where $h_e := (\vartheta^e - \vartheta^{e-1})$ and $t_e := (\vartheta - \vartheta^{e-1})/h_e$.

The boundary nodes must be treated separately. Over the first element, $e = 1$, for which $\vartheta \in [0, \vartheta^1]$, we have,

$$u(\vartheta) = u_0N_0^1(\vartheta) + u_1N_2^1(\vartheta) + u'_1N_3^1(\vartheta), \tag{6.20a}$$

$$v(\vartheta) = v'_0N_1^1(\vartheta) + v_1N_2^1(\vartheta) + v'_1N_3^1(\vartheta), \tag{6.20b}$$

$$\phi(\vartheta) = \phi_0N_0^1(\vartheta) + \phi_1N_2^1(\vartheta) + \phi'_1N_3^1(\vartheta). \tag{6.20c}$$

Similarly, over the last element, $e = N$, $\vartheta \in [\vartheta_{N-1}, \pi]$, we have,

$$u(\vartheta) = u_{N-1}N_0^N(\vartheta) + u'_{N-1}N_1^e(\vartheta) + u_NN_2^N(\vartheta), \tag{6.21a}$$

$$v(\vartheta) = v_{N-1}N_0^N(\vartheta) + v'_{N-1}N_1^N(\vartheta) + v'_NN_3^N(\vartheta), \tag{6.21b}$$

$$\phi(\vartheta) = \phi_{N-1}N_0^N(\vartheta) + \phi'_{N-1}N_1^N(\vartheta) + \phi_NN_2^N(\vartheta). \tag{6.21c}$$

The space for test functions are chosen to be the same as that of the dependent variables.

We now define the following integrals, which are the element Ω_e, contributions to the weak form,

$$F_i^e := \int_{\Omega_e} -c_g'(\phi)\tilde{b}^{\vartheta\vartheta}\partial_\vartheta\phi\partial_\vartheta N_i^e + cH\left(\Delta N_i^e\right) + \Big[\epsilon b^{\vartheta\vartheta}\phi_\vartheta^2 - 2\tilde{\gamma}H - p\Big]N_i^e + \lambda_z\Big(\cos\vartheta(n_r - 2Hu) - \sin\vartheta(n_\vartheta - 2Hv)\Big)\sqrt{g}\,d\vartheta, \tag{6.22a}$$

$$G_i^e := \int_{\Omega_e}\left\{\frac{1}{\sqrt{g}}\partial_\vartheta\left(\sqrt{g}^{\vartheta\vartheta}\right) - \sin(\vartheta)\cos(\vartheta)g^{\varphi\varphi} + \lambda_g\sin\vartheta\right\}N_i^e\sqrt{g}\,d\vartheta, \tag{6.22b}$$

$$\Psi_i^e := \int_{\Omega_e}\epsilon g^{\vartheta\vartheta}(\partial_\vartheta\phi)(\partial_\vartheta N_i^e) + \Big[W'(\phi) + \lambda + c'H^2 + c_g'K\Big]N_i^e\sqrt{g}\,d\vartheta, \tag{6.22c}$$

where $i \in \{0,1,2,3\}$.

The local contributions from the constraints are,

$$C_1^e := \int_{\Omega_e}(\sqrt{g} - \sin\vartheta)\,d\vartheta, \tag{6.22d}$$

$$C_2^e := \int_{\Omega_e}(\phi - \mu)\sqrt{g}\,d\vartheta, \tag{6.22e}$$

$$C_3^e := \int_{\Omega_e}(u\cos\vartheta - v\sin\vartheta)\sqrt{g}\,d\vartheta, \tag{6.22f}$$

$$C_4^e := \int_{\Omega_e}(\cos\vartheta)\sqrt{g}\,d\vartheta. \tag{6.22g}$$

We now define the local discretizations of the weak form. The elements with boundary nodes must be treated separately to impose boundary conditions. For the first element we define,

$$\mathbf{\Phi}_1^1 := \Big(F_0^1,\ G_1^1,\ \Psi_0^1\Big)_{1\times 3}^T, \tag{6.23a}$$

$$\mathbf{\Phi}_2^1 := \Big(F_2^1,\ F_3^1,\ G_2^1,\ G_3^1,\ \Psi_2^1, \Psi_3^1\Big)_{1\times 6}^T, \tag{6.23b}$$

$$\mathbf{C}^1 := \Big(C_1^1, C_2^1, C_3^1, C_4^1\Big)_{1\times 4}^T, \tag{6.23c}$$

and the following for the last element,

$$\mathbf{\Phi}_1^N := \Big(F_0^N,\ F_1^N,\ G_0^N,\ G_1^N,\ \Psi_0^N, \Psi_1^N\Big)_{1\times 6}^T, \tag{6.23d}$$

$$\mathbf{\Phi}_2^N := \Big(F_2^N,\ G_3^N,\ \Psi_2^N\Big)^T_{1\times 3}, \tag{6.23e}$$

$$\mathbf{C}^N := \Big(C_1^N, C_2^N, C_3^N, C_4^N\Big)^T_{1\times 4}. \tag{6.23f}$$

For all the other elements ($e \in \{2, 3, \cdots, N-1\}$),

$$\mathbf{\Phi}_1^e := \Big(F_0^e,\ F_1^e,\ G_0^e,\ G_1^e,\ \Psi_0^e, \Psi_1^e\Big)^T_{1\times 6}, \tag{6.23g}$$

$$\mathbf{\Phi}_2^e := \Big(F_2^e,\ F_3^e,\ G_2^e,\ G_3^e,\ \Psi_2^e, \Psi_3^e\Big)^T_{1\times 6}, \tag{6.23h}$$

$$\mathbf{C}^e := \Big(C_1^e, C_2^e, C_3^e, C_4^e\Big)^T_{1\times 4}. \tag{6.23i}$$

The local discretization of the weak form summarized by the previous system of equations, (6.23, are now assembled. This process is quite straightforward as the problem is one dimensional. We define the following vectors as a result of the assembly of equations and constraints,

$$\mathbf{\Phi} := \Big(\mathbf{\Phi}_1^1, \mathbf{\Phi}_2^1 + \mathbf{\Phi}_1^2, \mathbf{\Phi}_2^2 + \mathbf{\Phi}_1^3, \cdots, \mathbf{\Phi}_1^e + \mathbf{\Phi}_2^{e+1}, \cdots, \mathbf{\Phi}_2^{N-1} + \mathbf{\Phi}_1^N, \mathbf{\Phi}_2^N\Big)^T_{1\times 6N}, \tag{6.24a}$$

$$\mathbf{C} := \Big(\sum_e C_1^e, \sum_e C_2^e, \sum_e C_3^e, \sum_e C_4^e\Big)^T. \tag{6.24b}$$

The previous vectors can be combined to the following system,

$$\mathbf{F} := \Big(\mathbf{\Phi}, \mathbf{C}\Big)^T. \tag{6.24c}$$

The unknowns of the problem, namely, the nodal variables and the Lagrange multipliers are conveniently written as the following vector,

$$\mathbf{y} = \Big(\mathbf{y}_0, \mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_{N-1}, \mathbf{y}_N, \boldsymbol{\ell}\Big)^T. \tag{6.25}$$

The discretized problem can be stated succinctly as,

$$\mathbf{F}(\mathbf{y}, \boldsymbol{\lambda}) = \mathbf{0}, \tag{6.26}$$

where $\boldsymbol{\lambda}$ contains all the control parameters of the system. We treat this system as a bifurcation problem and perform path continuation using methods explained in section (6.2).

CHAPTER 7

COMPUTATIONS - STABILITY

In this chapter, we present a numerical scheme to assess stability of the computed equilibria . It is important to note that the hessian matrix used in Newton iteration while computing equilibria (discussed in the previous chapter) is only the *axisymmetric* contribution to the full hessian. That is, it is the second variation of the energy with respect to only axisymmetric perturbations.

To determine stability, the positive definiteness of the hessian should be established with respect to both axisymmetric and non-axisymmetric perturbations. With an explicit expression for the second variation, (4.19), at hand, the discretized hessian may be obtained by suitably discretizing the system. We follow the work of Wohlever *et. al.* [66] and use a Fourier-Galerkin approach to discretize the hessian of the lipid vesicle problem. In this method, the perturbations in the azimuthal direction φ are expanded in terms of $2M$ Fourier modes - sines and cosines functions and the meridional direction is discretized in terms of N Hermite cubic elements. With four unknown variables (two each for the normal variation w and concentration variation ψ) per node, $N+1$ nodes in the finite element discretization and $2M$ sines and cosines per node, the hessian matrix is of the order $12NM \times 12NM$. Directly assembling the hessian and computing its eigen values would be prohibitively expensive. For example, for a discretization with $N = 100$ and $M = 100$, the hessian will be of the order of $10^5 \times 10^5$.

Computations become more tractable if we recognize that axisymmetry of the equilibrium solutions renders the hessian with lots of zero entries. Using tools from group representation theory it is possible to construct a basis for the hessian, called a *symmetry adapted basis*, in which the matrix is block diagonalized. Each such a block can be then assembled independently. The stability is determined by the

computing the eigenvalues of each block. This method not only makes it trivial to parallelize computations, but it also has the added advantage of considerably reducing the cost of eigenvalue computations.

In the following section we briefly summarize the technique of computing the symmetry adapted basis using tools from group representation theory and projection operators. Details can be found in [4], [32], [18], [66].

7.1 Block Diagonalization and Symmetry Adapted Basis

We fist recall a few basic facts from group representation theory.

7.1.1 Group Representation Theory

Definition 13 (Group). *A set G with a binary operation $\cdot : G \times G \to G$ (usually written as the pair, $(G, \cdot)$, is said to be a group if the following properties hold:*

1. *There exists an element $e \in G$, called the* identity element *such that $e \cdot g = g \cdot e = g$, for all $g \in G$.*
2. *For every $g \in G$ there is an* inverse element*, $g^{-1} \in G$ that satisfies $g^{-1} \cdot g = g \cdot g^{-1} = e$.*
3. *For all $g, h, k \in G$, the identity $(g \cdot h) \cdot k = g \cdot (h \cdot k)$ holds true.*

For convenience, the operation $\cdot$ will be dropped whenever clear from context.

Closely associated with the concept of group is the idea of *homomorphism*. These are mappings of group that preserve the group structure, that is,

Definition 14 (Homomorphism). *Let $(G, \cdot)$ and $(H, \times)$ be two groups. A mapping $f : G \to H$ is said to be a* homomorphism *iff*

$$f(g_1 \cdot g_2) = f(g_1) \times f(g_2), \ \forall \ g_1, g_2 \in G.$$

In physical applications, groups are most commonly conceived by their action on the physical variables of the system, which are usually elements of some vector space. The group elements themselves are, therefore, linear transformations. This idea has been abstracted to the concept of *group representation* or *representation*. For our purposes here it suffices to restrict ourselves to the special case when the group of linear transformations are orthogonal transformation. Such a representation is called an *orthogonal representations*. It can be shown [23], that finite groups and compact Lie groups always admit orthogonal representations. We now define an orthogonal representation of a group G,

Definition 15 (Action and Orthogonal Representation)**.** *Let V be a real vector space of dimension n and O_n be the space of all orthogonal $n \times n$ real matrices. An* orthogonal representation *of a group G* acting *on V is a homomorphism, $T : G \to O_n$. In other words, for every $g_1, g_2 \in G$ we have $T(g_1)T(g_2) = T(g_1 g_2)$.*

It follows that, $T(g^{-1}) = T^{-1}(g)$ and $T(e) = I$.

In general, an n dimensional representation can be "broken down" into smaller building blocks. This idea is expressed via the following two definition,

Definition 16. *Let T be an orthogonal representation of a group G acting on a vector space V. A subspace W of V is said to be* invariant *under the action of T if $T(g)\mathbf{w} \in W$ for all $g \in G$ and $\mathbf{w} \in W$.*

Definition 17 (Reducible and Irreducible Representations)**.** *A representation T is* reducible *if there is a proper invariant subspace W of V. Otherwise T is said to be* irreducible.

Of special interest are irreducible representations that commute with identity,

Definition 18 (Absolutely Irreducible Representation)**.** *An irreducible representation is called* absolutely irreducible *if the only transformations that commute*

with $T(g) \in O_n$ are scalar multiples of the identity transformation on V.

7.1.2 Symmetry, Equivariance and Block Diagonalization

The symmetry of a vector $\mathbf{u} \in V$ is characterized by its *isotropy group*, noted in chapter (3). We define it again here, but this time in the context of representation theorey. For a given representation T of G, the isotropy group of a vector $\boldsymbol{u}$, is defined as follows,

Definition 19 (Isotropy Subgroup)**.** *A subgroup $\Sigma_{\boldsymbol{u}}$ of G defined by*

$$\Sigma_{\boldsymbol{u}} := \{g \in G \mid T_g \boldsymbol{u} = \boldsymbol{u}\}, \tag{7.1}$$

is called an isotropy subgroup *of G.*

The *fixed point set* for the representation is defined as,

Definition 20 (Fixed Point Set)**.** *Let Σ be a subgroup of G. The* Σ-fixed point set*, V_Σ is defined as*

$$V_\Sigma := \{\boldsymbol{u} \in V \mid T_g \boldsymbol{u} = \boldsymbol{u}, \forall g \in \Sigma\}. \tag{7.2}$$

It is easy to show [23] that V_Σ is an invariant subspace of V under the action of Σ.

Mathematically, the notion of symmetry may be expressed in terms of equivariance of the governing equations of a physical system. Since we are dealing problems that are framed in the context of bifurcation, λ in the following will represent the bifurcation parameter. We now define the notion of equivariance.

Definition 21 (Equivariance)**.** *A mapping $\mathbf{f} : V \times R \to V$ is said to be* equivariant *under the action of T if*

$$T_g \mathbf{f}(\boldsymbol{u}, \lambda) = \mathbf{f}(T_g \boldsymbol{u}, \lambda) \ \ \forall g \in G. \tag{7.3}$$

Assume that Σ is an isotropy group of a vector $\mathbf{u}$ and V_Σ is the corresponding fixed point set. Let us further assume that $\mathbf{f}$ is equivariant with respect to the representation T. Then, for every $g \in \Sigma$ and $(\mathbf{u}, \lambda) \in V_\Sigma \times \mathbb{R}$, we have,

$$T_g \mathbf{f}(\mathbf{u}, \lambda) = \mathbf{f}(T_g \mathbf{u}, \lambda) = \mathbf{f}(\mathbf{u}, \lambda). \tag{7.4}$$

Differentiating the previous equation with respect to $\boldsymbol{u}$, we have the following communtation relation between the hessian, $\mathbf{f_u}$, and the transformation, T_g,

$$T_g \mathbf{f_u}(\mathbf{u}, \lambda) = \mathbf{f_u}(\mathbf{u}, \lambda) T_g. \tag{7.5}$$

If the representation T is reducible, it can be shown that [18] the previous commutation relation leads to block diagonalization of the hessian.

7.1.3 Projection Operator Theory and Symmetry Adapted Basis

Block diagonalization of the hessian may be explicitly performed via the projection operators [18]. It is common to develop the theory of projection operators in the context of complex vector spaces. However there are fundamental differences in the theory of irreducible representations of real and complex spaces, as noted by Aston [4]. By restricting oneself to absolutely irreducible representations, the results developed for complex vectors spaces can be directly applied to real vector spaces. For this reason, we shall consider only real irreps that are absolutely irreducible. We refer the reader to the following works for details on this topic: [4, 23, 32].

Any reducible representation, T_g, can be decomposed into a direct sum of irreducible representations [18] $\gamma_g^{(\mu)}$, where $\mu = 1, 2, \cdots, p$.

$$T_g = \bigoplus_{\mu=1}^{p} c_\mu \gamma_g^{(\mu)}, \tag{7.6}$$

here, p is the number of distinct irreducible representations contained in T and c_μ is the number of copies of the irrep $\gamma^{(\mu)}$. We note the following formula for c_μ,

$$c_\mu = \int_G tr(\gamma_g^{(\mu)})^* tr(T_g)\, d\sigma(g), \tag{7.7}$$

where $tr(\cdot)$ represents the trace of the appropriate matrix and $d\sigma(g)$ is the Haar measure on the group G. For finite groups, the integral is replaced by a summation over the group.

The space V can also be resolved into mutually orthogonal T-invariant subspaces $V^{(\mu)}$ as follows,

$$V = \bigoplus_{\mu=1}^{p} V^{(\mu)}. \tag{7.8}$$

In the case when the representations $\gamma^{(\mu)}$ are *absolutely irreducible*, we can further decompose $V^{(\mu)}$ as follows,

$$V^{(\mu)} = \bigoplus_{i=1}^{m_\mu} V_i^{(\mu)}. \tag{7.9}$$

The dimension of each subspace $V^{(\mu)}$ is given be

$$n_\mu = m_\mu \int_G tr(\gamma_g^{(\mu)})^* tr(T_g)\, d\sigma(g) = m_\mu c_\mu, \tag{7.10}$$

where m_μ denote the dimension of the representation $\gamma^{(\mu)}$. We define the following projection operators,

Definition 22 (Projection Operators)**.** *If G is a compact Lie group, then the projection operator $\mathcal{P}^\mu$, $\mathcal{P}_j^\mu$ are defined as follows,*

$$\mathcal{P}^\mu := m_\mu \int_G tr(\gamma_g^{(\mu)})^* T_g\, d\sigma(g), \tag{7.11}$$

$$\mathcal{P}_j^\mu := m_\mu \int_G [\gamma_g^{(\mu)}]_{j1}^* T_g\, d\sigma(g), \tag{7.12}$$

where $[\gamma_g^{(\mu)}]_{j1}$ is the $j1^{th}$ entry in the matrix $[\gamma_g^{(\mu)}]$.

It can be shown that [18] the following relation between the projection operators and subspaces holds,

$$V_j^{(\mu)} = \mathcal{P}_j^{\mu} \circ V_1^{(\mu)}. \tag{7.13}$$

The bases of $V_j^{(\mu)}$ are called the symmetry adapted bases. If this basis for V is chosen, the hessian matrix can be shown to have block-diagonalized form [18].

7.2 Discretizing the Hessian

We now discretize the hessian (including nonaxisymmetric variations) by expanding the variations in the azimuthal direction in terms of their Fourier modes and the meridonal direction using Hermite cubic elements Thus, the hessian is discretized using a Fourier-Galerkin scheme [66]. Let us first recall the explicit expression for the hessian from Chapter (4),

$$\mathcal{H}[w,\psi] = \int_{S^2} \Big(H_1[w,w] + H_2[w,\psi] + H_3[\psi,\psi] \Big) \sqrt{g}\, dA, \tag{7.14}$$

where H_1, H_2 and H_3 are symmetric bilinear operators on their respective arguments given by

$$\begin{aligned} H_1 = \frac{c}{2}(\Delta w)^2 + [c(5H^2 - K) - \tilde{\gamma} + \Delta c_g] w \Delta w + \Big[\epsilon \phi^{\alpha}\phi^{\beta} - 2Hc\tilde{b}^{\alpha\beta} - \nabla^{\alpha\beta} c_g \Big] w \nabla_{\alpha\beta} w \\ + 2\Big[H\nabla^{\alpha}(cH) - b^{\alpha\beta}(cH)_{\beta} - \frac{K}{2}\nabla^{\alpha} c_g \Big] w \nabla_{\alpha} w \\ + \Big[2\tilde{\gamma}K + c(8H^4 - 10H^2K + 2K^2) + 2\epsilon H b^{\alpha\beta}\phi_{\alpha}\phi_{\beta} - 3\epsilon K \phi_{\alpha}\phi^{\alpha} + 2Hp \Big] w^2, \end{aligned} \tag{7.15a}$$

$$\begin{aligned} H_2 = 2 \Big\{ -2\epsilon \left[\nabla_{\alpha}(b^{\alpha\beta} w \phi_{\beta}) - \nabla^{\alpha}(Hw)\phi_{\alpha} \right] + c' H \Big[\Delta w + 2(2H^2 - K) w \Big] + \\ c_g' \left[\tilde{b}^{\alpha\beta} \nabla_{\alpha\beta} w + 2KHw \right] \Big\} \psi, \end{aligned} \tag{7.15b}$$

$$H_3 = -\epsilon \psi \Delta \psi + (W'' + c'' H^2 + c_g'' K)\psi^2, \tag{7.15c}$$

such that the variations w and ψ satisfy the following constraints,

$$\int_\omega Hw\, da = 0, \tag{7.16}$$

$$\int_\omega [\psi - 2H\phi w]\, da = 0. \tag{7.17}$$

We divide the vesicle into N ring elements, and the variations w and ψ are approximated via Hermite cubics along ϑ and by M Fourier sine and cosine modes along the azimuthal direction, φ. That is, on the ring $\Omega_e \times [0, 2\pi]$, we have,

$$w(\vartheta, \varphi) = \bar{w}(\vartheta) + \sum_{m=1}^{M} \left[\hat{w}_m(\vartheta)\cos(m\varphi) + \tilde{w}_m(\vartheta)\sin(m\varphi)\right], \tag{7.18a}$$

$$\psi(\vartheta, \varphi) = \bar{\psi}(\vartheta) + \sum_{m=1}^{M} \left[\hat{\psi}_m(\vartheta)\cos(m\varphi) + \tilde{\psi}_m(\vartheta)\sin(m\varphi)\right], \tag{7.18b}$$

where $\bar{w}$, $\hat{w}$, $\tilde{w}$ and $\bar{\psi}$, $\hat{\psi}$, $\tilde{\psi}$ are defined in terms of the Hermite cubics (6.19) as follows,

$$\bar{w}(\vartheta) = \bar{w}_{e-1}N_0^e(\vartheta) + \bar{w}'_{e-1}N_1^e(\vartheta) + \bar{w}_e N_2^e(\vartheta) + \bar{w}'_e N_3^e(\vartheta), \tag{7.19a}$$

$$\hat{w}_m(\vartheta) = \hat{w}_{m,e-1}N_0^e(\vartheta) + \hat{w}'_{m,e-1}N_1^e(\vartheta) + \hat{w}_{m,e}N_2^e(\vartheta) + \hat{w}'_{m,e}N_3^e(\vartheta), \tag{7.19b}$$

$$\tilde{w}_m(\vartheta) = \tilde{w}_{m,e-1}N_0^e(\vartheta) + \tilde{w}'_{e-1}N_1^e(\vartheta) + \tilde{w}_{m,e}N_2^e(\vartheta) + \tilde{w}'_{m,e}N_3^e(\vartheta), \tag{7.19c}$$

and

$$\bar{\psi}(\vartheta) = \bar{\psi}_{e-1}N_0^e(\vartheta) + \bar{\psi}'_{e-1}N_1^e(\vartheta) + \bar{\psi}_e N_2^e(\vartheta) + \bar{\psi}'_e N_3^e(\vartheta), \tag{7.20a}$$

$$\hat{\psi}_m(\vartheta) = \hat{\psi}_{m,e-1}N_0^e(\vartheta) + \hat{\psi}'_{m,e-1}N_1^e(\vartheta) + \hat{\psi}_{m,e}N_2^e(\vartheta) + \hat{\psi}'_{m,e}N_3^e(\vartheta), \tag{7.20b}$$

$$\tilde{\psi}_m(\vartheta) = \tilde{\psi}_{m,e-1}N_0^e(\vartheta) + \tilde{\psi}'_{m,e-1}N_1^e(\vartheta) + \tilde{\psi}_{m,e}N_2^e(\vartheta) + \tilde{\psi}'_{m,e}N_3^e(\vartheta). \tag{7.20c}$$

7.3 Symmetry Adapted Basis for Axisymmetric Solutions

Using the theory presented in section (7.1.3), we compute the symmetry adapted basis for the hessian in the case when the equilibria are known to be axisymmetric, *i.e.,* whose symmetry group is $O(2)$. First we recall the irreducible representations of $O(2)$.

7.3.1 Irreducible Representations of $O(2)$

The group of orthogonal transformations of the real plane, $O(2)$, is a *compact lie group* that is generated by the elements r_θ, the rotation of the plane by $\theta \in \mathbb{R}/2\pi\mathbb{Z} \cong S^1$ and s, reflection across a diameter.

Every irreducible representation of $O(2)$ falls in to one of the following countably many possibilities, [66, 18],

$$\gamma_\theta^{(1)} = \gamma_s^{(1)} = 1, \tag{7.21}$$

$$\gamma_\theta^{(2)} = -\gamma_s^{(2)} = 1, \tag{7.22}$$

$$\gamma_\theta^{(2+h)} = \begin{pmatrix} \cos h\theta & \sin h\theta \\ -\sin h\theta & \cos h\theta \end{pmatrix}, \gamma_s^{(2+h)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{7.23}$$

where as before, $\theta \in \mathbb{R}/2\pi\mathbb{Z}$, $h = 1, 2, 3, \cdots$. The first two representations are one-dimensional and the rest are two-dimensional. In computations, discretization forces only a finite number of these representations appear.

The invariant Haar measure on $O(2)$ is $\frac{1}{4\pi}d\theta$, [23], which makes the the integrals in the projection operators,

$$\int_G d\sigma(g) = \frac{1}{4\pi}\int_0^{2\pi} d\theta. \tag{7.24}$$

7.3.2 Representation of $O(2)$ for Multiphase Membranes

In this section we compute the representation of $O(2)$ on the space of discretized variations. Let us first note the following definitions for the nodal variables,

$$\mathbf{w}_0 := \left(\bar{w}_0, \hat{w}_{1,0}, \tilde{w}_{1,0}, \hat{w}'_{1,0}, \tilde{w}'_{1,0}, \cdots, \hat{w}_{M,0}, \tilde{w}_{M,0}, \hat{w}'_{M,0}, \tilde{w}'_{M,0}\right)^T_{1\times(4M+1)}, \tag{7.25}$$

$$\mathbf{w}_e := \left(\bar{w}_e, \bar{w}'_e, \hat{w}_{1,e}, \tilde{w}_{1,e}, \hat{w}'_{1,e}, \tilde{w}'_{1,e}, \cdots, \hat{w}_{M,e}, \tilde{w}_{M,e}, \hat{w}'_{M,e}, \tilde{w}'_{M,e}\right)^T_{1\times(4M+2)}, \tag{7.26}$$

$$\mathbf{w}_N := \left(\bar{w}_N, \hat{w}_{1,N}, \tilde{w}_{1,N}, \hat{w}'_{1,N}, \tilde{w}'_{1,N}, \cdots, \hat{w}_{M,N}, \tilde{w}_{M,N}, \hat{w}'_{M,N}, \tilde{w}'_{M,N}\right)^T_{1\times(4M+1)}, \tag{7.27}$$

$$\boldsymbol{\psi}_0 := \left(\bar{\psi}_0, \hat{\psi}_{1,0}, \tilde{\psi}_{1,0}, \hat{\psi}'_{1,0}, \tilde{\psi}'_{1,0}, \cdots, \hat{\psi}_{M,0}, \tilde{\psi}_{M,0}, \hat{\psi}'_{M,0}, \tilde{\psi}'_{M,0}\right)^T_{1\times(4M+1)}, \tag{7.28}$$

$$\boldsymbol{\psi}_e := \left(\bar{\psi}_e, \bar{\psi}'_e, \hat{\psi}_{1,e}, \tilde{\psi}_{1,e}, \hat{\psi}'_{1,e}, \tilde{\psi}'_{1,e}, \cdots, \hat{\psi}_{M,e}, \tilde{\psi}_{M,e}, \hat{\psi}'_{M,e}, \tilde{\psi}'_{M,e}\right)^T_{1\times(4M+2)}, \tag{7.29}$$

$$\boldsymbol{\psi}_N := \left(\bar{\psi}_N, \hat{\psi}_{1,N}, \tilde{\psi}_{1,N}, \hat{\psi}'_{1,N}, \tilde{\psi}'_{1,N}, \cdots, \hat{\psi}_{M,N}, \tilde{\psi}_{M,N}, \hat{\psi}'_{M,N}, \tilde{\psi}'_{M,N}\right)^T_{1\times(4M+1)}. \tag{7.30}$$

Putting these together,

$$\mathbf{w} = \left(\mathbf{w}_0, \mathbf{w}_1, \cdots, \mathbf{w}_e, \cdots, \mathbf{w}_{N-1}, \mathbf{w}_N\right)^T \in \mathbb{R}^{(4MN+4M+2N)} =: W, \tag{7.31a}$$

$$\boldsymbol{\psi} = \left(\boldsymbol{\psi}_0, \boldsymbol{\psi}_1, \cdots, \boldsymbol{\psi}_e, \cdots, \boldsymbol{\psi}_{N-1}, \boldsymbol{\psi}_N\right)^T \in \mathbb{R}^{(4MN+4M+2N)} =: \Psi. \tag{7.31b}$$

We now define a representation of $O(2)$ on the spaces W and Ψ, using the following relations,

$$T_\alpha w(\vartheta, \varphi) := w(\vartheta, \varphi+\alpha),\ T_{s\alpha} w(\vartheta, \varphi) := w(\vartheta, -\varphi-\alpha),\ \text{for all } \alpha \in [0, 2\pi], \tag{7.32a}$$

$$T_\alpha \psi(\vartheta, \varphi) := \psi(\vartheta, \varphi+\alpha),\ T_{s\alpha} \psi(\vartheta, \varphi) := \psi(\vartheta, -\varphi-\alpha),\ \text{for all } \alpha \in [0, 2\pi]. \tag{7.32b}$$

The previous equations induce the following relations on the discretizations,

$$T_\alpha w = \bar{w}(\vartheta) + \sum_{m=1}^{M} \left[\hat{w}_m(\vartheta) \cos\left(m(\varphi+\alpha)\right) + \tilde{w}_m(\vartheta) \sin\left(m(\varphi+\alpha)\right)\right], \tag{7.33a}$$

$$T_{s\alpha} w = \bar{w}(\vartheta) + \sum_{m=1}^{M} \left[\hat{w}_m(\vartheta) \cos\left(m(-\varphi-\alpha)\right) + \tilde{w}_m(\vartheta) \sin\left(m(-\varphi-\alpha)\right)\right]. \tag{7.33b}$$

Similar relations for ψ hold.

Thus we have the following matrices as the representation of $O(2)$ on the discretized space W,

$$\hat{T}^w_\alpha = \begin{pmatrix} A_\alpha & O & O & \cdots & O & O \\ O & B_\alpha & O & \cdots & O & O \\ O & O & B_\alpha & \cdots & O & O \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ O & O & O & \cdots & B_\alpha & O \\ O & O & O & \cdots & O & A_\alpha \end{pmatrix}, \tag{7.34}$$

$$\hat{T}^{w}_{s\alpha} = \begin{pmatrix} A_{s\alpha} & O & O & \cdots & O & O \\ O & B_{s\alpha} & O & \cdots & O & O \\ O & O & B_{s\alpha} & \cdots & O & O \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ O & O & O & \cdots & B_{s\alpha} & O \\ O & O & O & \cdots & O & A_{s\alpha} \end{pmatrix}, \tag{7.35}$$

where A_α, $A_{s\alpha}$ are each $(4M+1)\times(4M+1)$ matrices and B_α, $B_{s\alpha}$ are $(4M+2)\times(4M+2)$ matrices given as follows,

$$A_\alpha = \begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & G_\alpha & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{0} & \mathbf{O} & G_{2\alpha} & \cdots & \mathbf{O} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{O} & \mathbf{O} & \cdots & G_{M\alpha} \end{pmatrix}, \; B_\alpha = \begin{pmatrix} \mathbf{I} & \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & G_\alpha & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & G_{2\alpha} & \cdots & \mathbf{O} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{O} & \mathbf{O} & \mathbf{O} & \cdots & G_{M\alpha} \end{pmatrix}, \tag{7.36}$$

$$A_{s\alpha} = \begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & G_{s\alpha} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{0} & \mathbf{O} & G_{2s\alpha} & \cdots & \mathbf{O} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{O} & \mathbf{O} & \cdots & G_{Ms\alpha} \end{pmatrix}, \; B_{s\alpha} = \begin{pmatrix} \mathbf{I} & \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & G_{s\alpha} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & G_{2s\alpha} & \cdots & \mathbf{O} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{O} & \mathbf{O} & \mathbf{O} & \cdots & G_{Ms\alpha} \end{pmatrix}, \tag{7.37}$$

where G_θ and $G_{s\theta}$ are defined by

$$G_\theta := \begin{pmatrix} \gamma_\alpha & O \\ O & \gamma_\alpha \end{pmatrix}, \; G_{s\theta} := \begin{pmatrix} \gamma_{s\alpha} & O \\ O & \gamma_{s\alpha} \end{pmatrix}. \tag{7.38}$$

We get another copy of this representation in the form of $\hat{T}^{\psi}$ for the representation of $O(2)$ on Ψ. By taking the direct sum of the above two representations, we obtain

a representation of $O(2)$ on $V := W \oplus \Psi$, the discretized nodal space.

$$\hat{T}_\alpha = \left(\begin{array}{c|c} \hat{T}^w_\alpha & O \\ \hline O & \hat{T}^\psi_\alpha \end{array}\right), \quad \hat{T}_{s\alpha} = \left(\begin{array}{c|c} \hat{T}^w_{s\alpha} & O \\ \hline O & \hat{T}^\psi_{s\alpha} \end{array}\right). \tag{7.39}$$

7.3.3 Symmetry Adapted Basis

Writing the projection operators as defined in section 7.1.3 on the space $V = W \oplus \Psi$

$$\mathcal{P}^1 = \frac{1}{4\pi} \int_{-\pi}^{\pi} \left(\hat{T}_\alpha + \hat{T}_{s\alpha}\right) d\alpha, \tag{7.40}$$

$$\mathcal{P}^1 = \left(\begin{array}{c|c} P^1 & O \\ \hline O & P^1 \end{array}\right), \tag{7.41}$$

where,

$$P^1 = \begin{pmatrix} I_1 & O & \cdots & O & O \\ O & I_2 & \cdots & O & O \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ O & O & \cdots & I_2 & O \\ O & O & \cdots & O & I_1 \end{pmatrix}, \tag{7.42}$$

where

$$I_1 = \begin{pmatrix} 1 & O_{1\times 4M} \\ O_{4M\times 1} & O_{4M\times 4M} \end{pmatrix}, \quad I_2 = \begin{pmatrix} I_{2\times 2} & O_{2\times 4M} \\ O_{4M\times 2} & O_{4M\times 4M} \end{pmatrix}. \tag{7.43}$$

Recall that the invariant subspace, $V^{(1)}$ is the range of the operator $\mathcal{P}^1$. The symmetry adapted basis for this subspace are the column vectors of the projection operator. Therefore,

$$V^{(1)} = V^{(1)}_w \oplus V^{(1)}_\psi, \tag{7.44}$$

$$V^{(1)}_w = \text{Span}\Big\{\bar{w}_0, \bar{w}_1, \bar{w}'_1, \bar{w}_2, \bar{w}'_2, \cdots, \bar{w}_e, \bar{w}'_e, \cdots, \bar{w}_{N-1}, \bar{w}'_{N-1}, \bar{w}_N\Big\}, \tag{7.45}$$

$$V^{(1)}_\psi = \text{Span}\Big\{\bar{\psi}_0, \bar{\psi}_1, \bar{\psi}'_1, \bar{\psi}_2, \bar{\psi}'_2, \cdots, \bar{\psi}_e, \bar{\psi}'_e, \cdots, \bar{\psi}_{N-1}, \bar{\psi}'_{N-1}, \bar{\psi}_N\Big\}. \tag{7.46}$$

In other words, the space $V^{(1)}$ is spanned by axisymmetric modes. The corresponding axisymmetric block is the same as the one used for computing the axisymmetric solutions.

The projection operator $\mathcal{P}^2$, corresponding to the second one-dimensional representation is,

$$\mathcal{P}^2 = \frac{1}{4\pi}\int_{-\pi}^{\pi}\left(\hat{T}_\alpha - \hat{T}_{s\alpha}\right)d\alpha = O. \tag{7.47}$$

Since this operator vanishes identically, the corresponding invariant subspace is trivial, $V^{(2)} = 0$.

Now, for the two-dimensional representations,

$$\mathcal{P}_1^{(2+h)} = \frac{2}{4\pi}\int_{-\pi}^{\pi}\cos(h\alpha)\left(\hat{T}_\alpha + \hat{T}_{s\alpha}\right)d\alpha, \tag{7.48}$$

$$\mathcal{P}_1^{(2+h)} = \left(\begin{array}{c|c} P_1^{2+h} & O \\ \hline O & P_1^{2+h} \end{array}\right), \tag{7.49}$$

where

$$P_1^{2+h} := \begin{pmatrix} J_h & O & \cdots & O & O \\ O & K_h & \cdots & O & O \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ O & O & \cdots & K_h & O \\ O & O & \cdots & O & J_h \end{pmatrix}, \tag{7.50}$$

where,

$$J_h := \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \begin{array}{ccccccccc} & & & & & 2h & 2h+1 & 2h+2 & 2h+3 \end{array} \\ \begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \mathbf{1} & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & \mathbf{1} & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix} \end{array}, \tag{7.51}$$

$$K_h := \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \begin{array}{ccccccccc} & & & & & 2h+1 & 2h+2 & 2h+3 & 2h+4 \end{array} \\ \begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \mathbf{1} & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & \mathbf{1} & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix} \end{array}, \tag{7.52}$$

The projection operators $\mathcal{P}^{(2+h)}$ correspond to a two-dimensional absolutely irreducible representation. So, the subspace $V^{(2+h)}$ can be further decomposed (not necessarily uniquely) as $V_1^{(2+h)} \oplus V_2^{(2+h)}$. The range of $\mathcal{P}_1^{(2+h)}$ is the subspace $V_1^{(2+h)}$. Symmetry adapted basis are the columns of the projection operator. More

specifically,

$$V_1^{(2+h)} = W_1^{(2+h)} \oplus \Psi_1^{(2+h)}, \tag{7.53}$$

where,

$$W_1^{(2+h)} = \text{Span}\Big\{\hat{w}_{h,0}, \hat{w}'_{h,0}, \hat{w}_{h,1}, \hat{w}'_{h,1}, \cdots, \hat{w}_{h,e}, \hat{w}'_{h,e}, \cdots, \hat{w}_{h,N}, \hat{w}'_{h,N}\Big\}, \tag{7.54}$$

$$\Psi_1^{(2+h)} = \text{Span}\Big\{\hat{\psi}_{h,0}, \hat{\psi}'_{h,0}, \hat{\psi}_{h,1}, \hat{\psi}'_{h,1}, \cdots, \hat{\psi}_{h,e}, \hat{\psi}'_{h,e}, \cdots, \hat{\psi}_{h,N}, \hat{\psi}'_{h,N}\Big\}, \tag{7.55}$$

Using the symmetry adapted basis described above, the vector space V can be decomposed into invariant subspaces as follows,

$$V = V^{(1)} \oplus \bigoplus_{h=1}^{M} \Big(V_1^{(2+h)} \oplus V_2^{(2+h)}\Big). \tag{7.56}$$

7.3.4 Block Diagonalization of the Hessian

The discretized hessian matrix, when written in the symmetry adapted basis block diagonalizes. It can be shown [66], that the blocks corresponding to the subspaces $V_1^{(2+h)}$ and $V_2^{(2+h)}$ are identical. Therefore, it suffices to only assemble one of the blocks for checking stability. It is clear that block diagonalization offers a significant reduction in computational costs. An added benefit is the parallelizability of computations which can be achieved trivially by assembling each block independently.

Schematically, the block diagonalized hessian can be visualized as shown in figure (7.1). In this schematic, the block A is the axisymmetric block that is $4N \times 4N$. The blocks B_1 and B'_1 are identical and correspond to the invariant subspaces $V_1^{(3)}$ and $V_2^{(3)}$. Each of these subspaces is a $4(N+1)$ dimensional space, therefore the matrices B_1 and B'_1 are each $4(N+1) \times 4(N+1)$. Similarly $B_2 = B'_2$ is a $4(N+1) \times 4(N+1)$ matrix. Excluding the block A, there are M number of blocks (B_i), each appearing with an identical twin (B'_i).

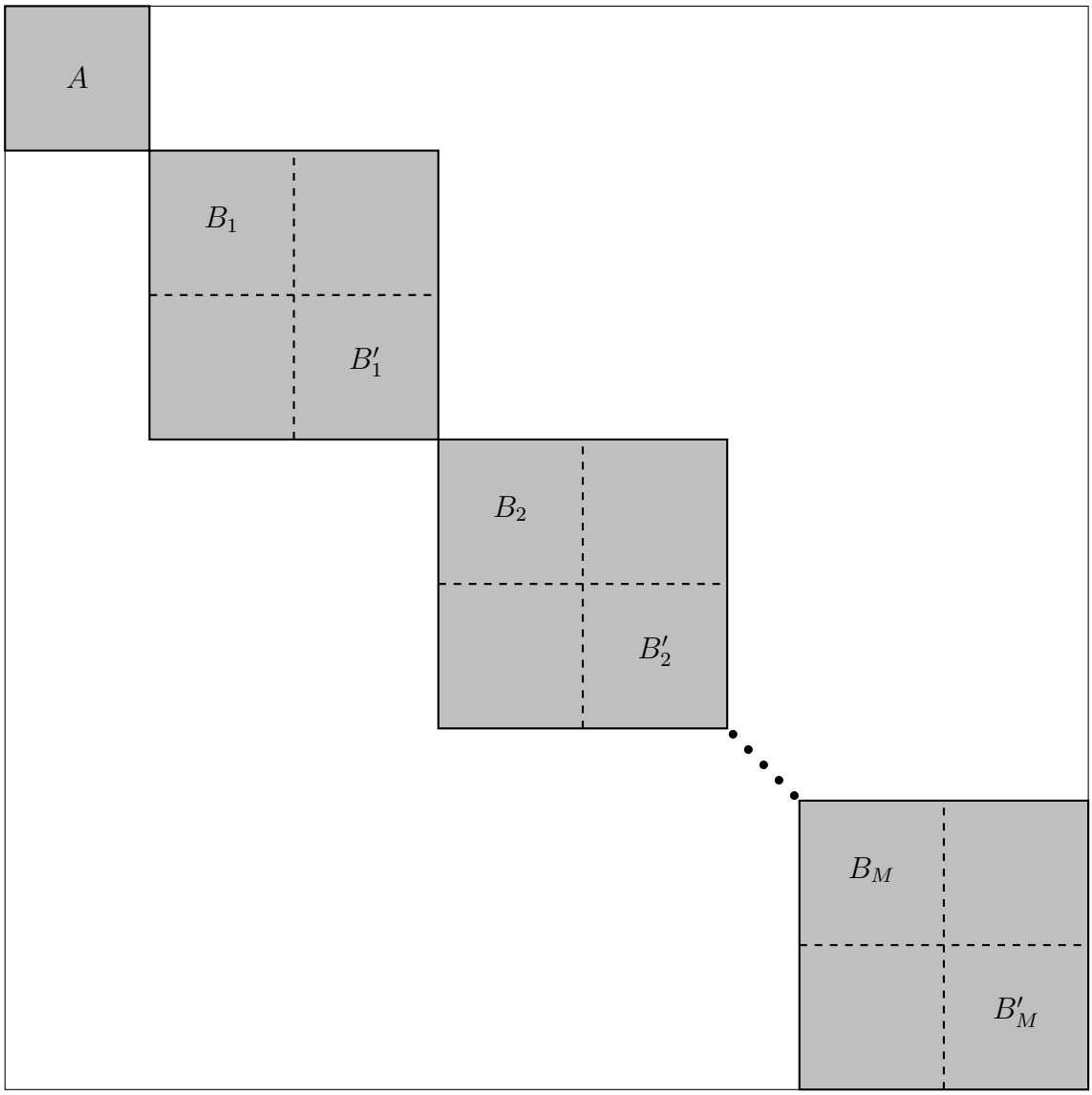


Figure 7.1: Schematic of the hessian when written in the symmetry adapted basis

It is therefore sufficient to only assemble the matrices $A, B_1, B_2, \cdots, B_M$ to determine stability. Due to the presence of constraints in the problem, we discretize their linearized equations (7.16) and (7.17). These are then used with the discretized hessian to determine stability. Each block is assembled along with the corresponding discretized linearized constraints and a constrained eigen value problem in solved using the method detailed in [29]. Arnoldi iterative solver (ARPACK) is used to accurately determine the lowest five eigen values in each block. Solution is considered unstable if a negative eigen value is detected in any one of the blocks.

CHAPTER 8

COMPUTATIONAL RESULTS

8.1 Introduction

In this chapter, we summarize computational results. Bifurcation diagrams are plotted using numerical path following on the discretized equations, (6.26) by treating the parameters of the system as the bifurcation variables. The stability of the branches are determined by assembling the individual blocks of the hessian as described in the previous chapter.

We start our continuation on the trivial branch and look for bifurcations from this branch. We use the characteristic equation (3.5) as a guide to search for bifurcation points. Branches corresponding to the modes $l = 1, 2, 3, 4$ are explored in this chapter.

8.1.1 First Mode: Symmetric Case

Studies on the Cahn-Hilliard equation [49] suggests that one expects phase separation only in the limit of ϵ being very small. However, choosing a small value for ϵ, the coefficient of the Laplace-Beltrami in (2.30b) is bad for numerical accuracy. Instead, we follow the strategy employed by Healey, *et. al.* [31, 30] of using the reciprocal of ϵ as a bifurcation parameter.

Figures (8.1-8.3) show the vesicle shapes for three particular choices of corresponding to $\epsilon = 1.0444$, $\epsilon = 0.1703$ and $\epsilon = 0.0062$, respectively. We also provide the mean curvature H and the phase field ϕ plotted as a function of the polar angle, ϑ, for convenience. Also shown in the bottom right corner is the bifurcation diagram. Note the considerable sharpening of the interface as $1/\epsilon$ is increased (correspondingly as ϵ is decreased). The number of elements (N) was chosen via

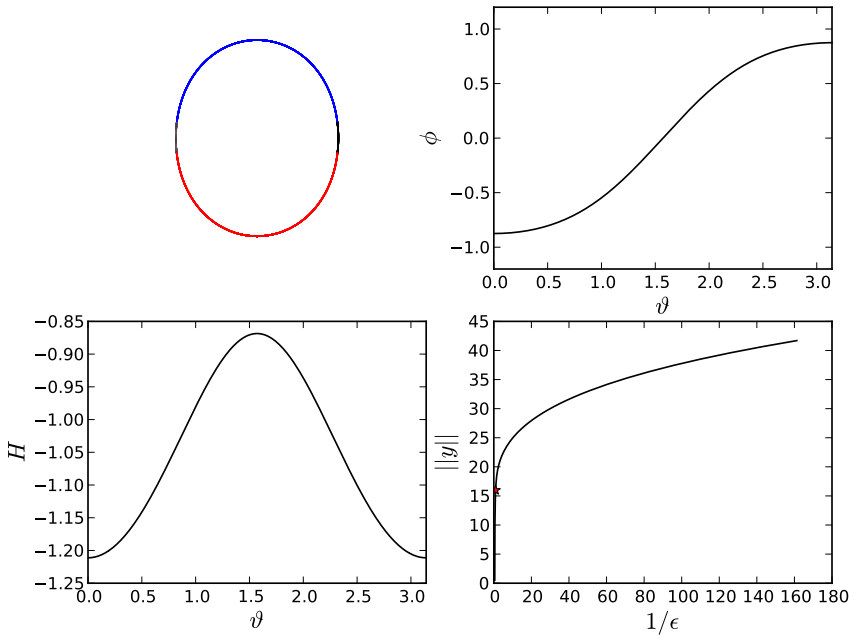


Figure 8.1: Symmetric First Mode for $\epsilon = 1.0444$

numerical exploration until sufficient convergence of results was obtained. For the above case, we find $N = 300$ to work satisfactorily. Other fixed parameters and their corresponding values are as follows: bending stiffness (independent of ϕ) $c = 1$, pressure $p = 1.0$, $\mu = 0$. Recall that μ represents the average value of the concentration on the membrane. Setting this variable to zero gives us symmetric shapes.

We note that there is no "pinching effect" at the phase boundaries in all the previous figures. This suggests that the membrane is quite stiff and its bending stiffness, which has been set to $c = 1$, is relatively large. In order to soften the membrane and improve the pinching effect, we decrease the bending stiffness. Accordingly, we fix $\epsilon = 0.0062$ and restart our continuation by decreasing c. This strategy of freezing a set of parameters and "switching on" a relevant parameter to explore the parameter space via numerical continuation has been successfully used

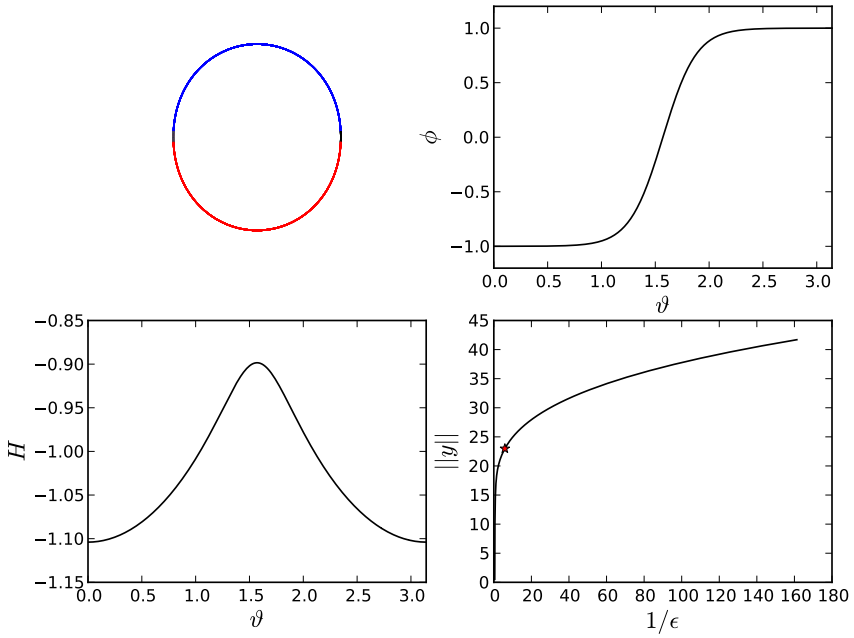


Figure 8.2: Symmetric First Mode for $\epsilon = 0.1703$

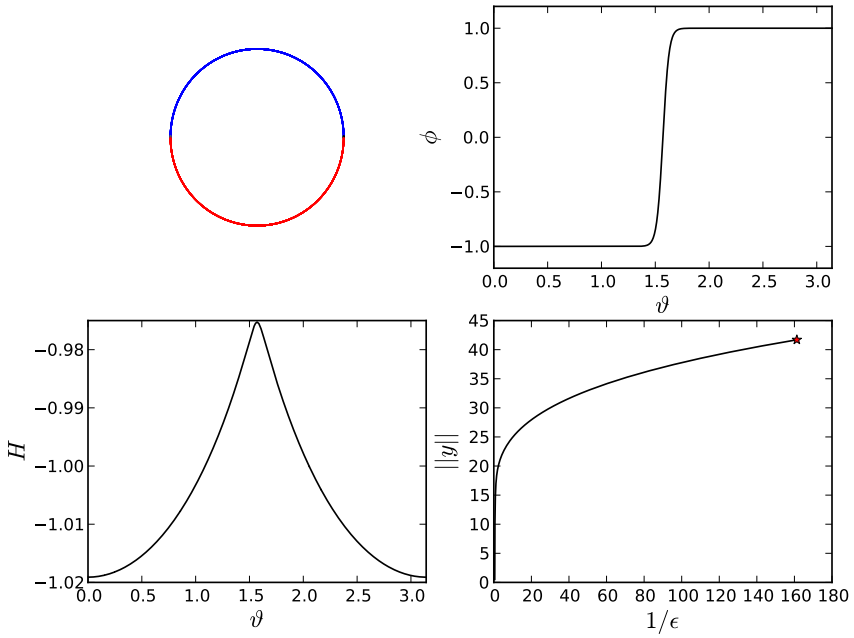


Figure 8.3: Symmetric First Mode for $\epsilon = 0.0062$

by Healey, *et al* [31, 30] in problems of nonlinear elasticity. We inform our choice of continuation parameters by using experiments of Baumgart, *et al* [5] as a visual guide. Our interest is to generate numerical representation of pinched solutions found in their work (cf. Fig(2.2)). A schematic for this strategy is shown in figure (8.4).

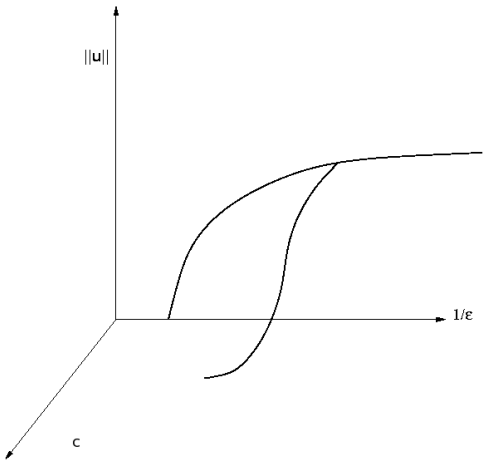


Figure 8.4: Schematic of the continuation scheme

Figures (8.5-8.7) show the vesicle shapes as the bending stiffness, c, is decreased in the following steps, $c = 0.9523$, $c = 0.0488$, $c = 0.0069$, respectively. The bending stiffness is still treated to be independent of the concentration field. In these cases, we observe that the pinching effect at the phase boundaries is noticeable, albeit, marginal.

We now continue in the pressure variable figures (8.8)-(8.11)), freezing the other variables. In particular, we fix $c = 0.0069$ (the last value in the previous continuation). As the pressure, p, is changed, we note a limit point in the bifurcation diagram. That is, for a given value of p there are two possible shapes corresponding to the two branches across the limit point. Interestingly, we find that one branch generates the pinched states observed in experiments. One instance, of such a shape for which $p = 1.06123$ is shown in Fig. (8.11).

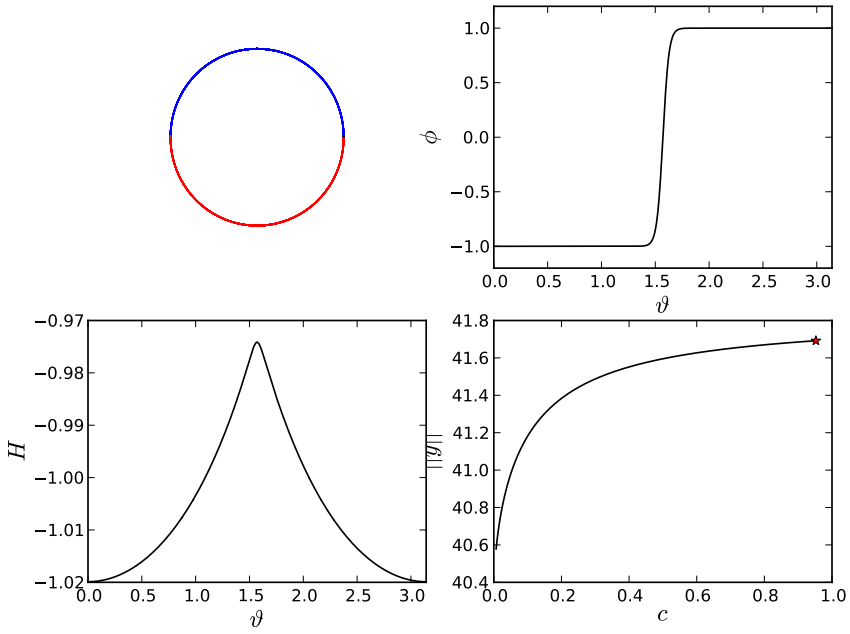


Figure 8.5: Symmetric First Mode for $c = 0.9523$

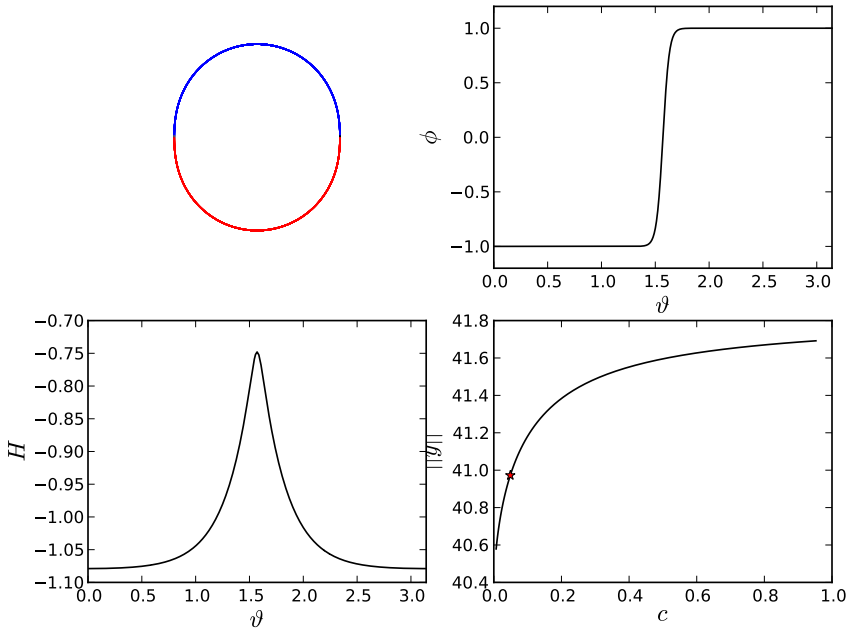


Figure 8.6: Symmetric First Mode for $c = 0.0488$

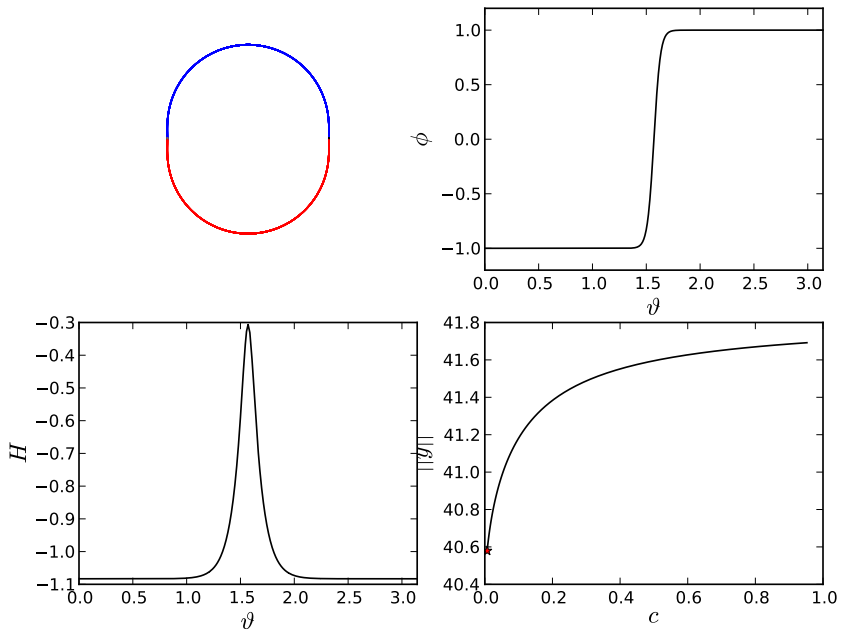


Figure 8.7: Symmetric First Mode for $c = 0.0069$

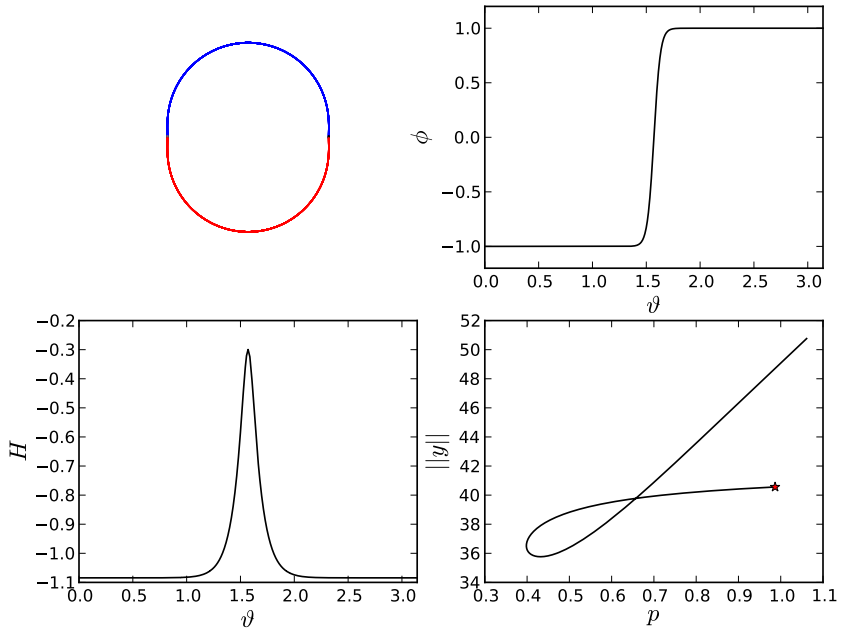


Figure 8.8: Symmetric First Mode for $p = 0.9867$

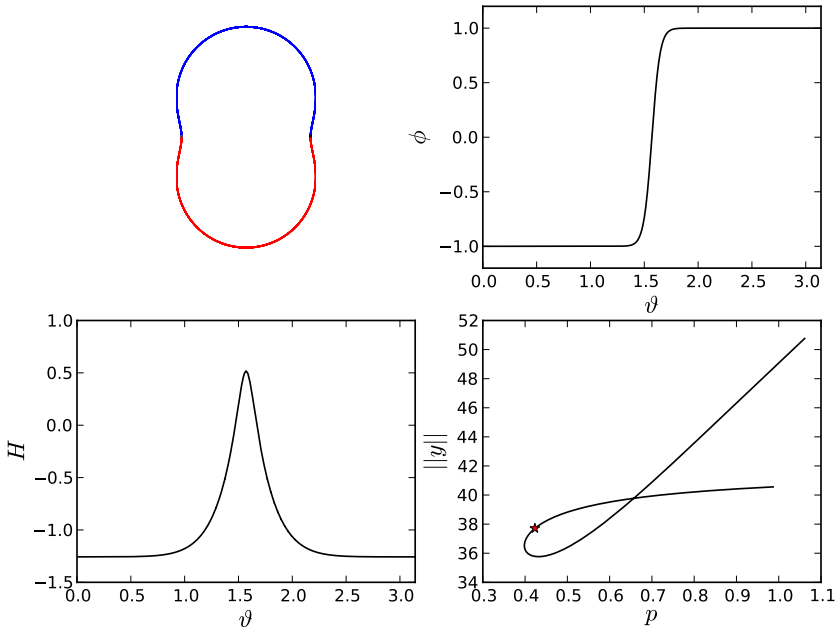


Figure 8.9: Symmetric First Mode for $p = 0.4231$

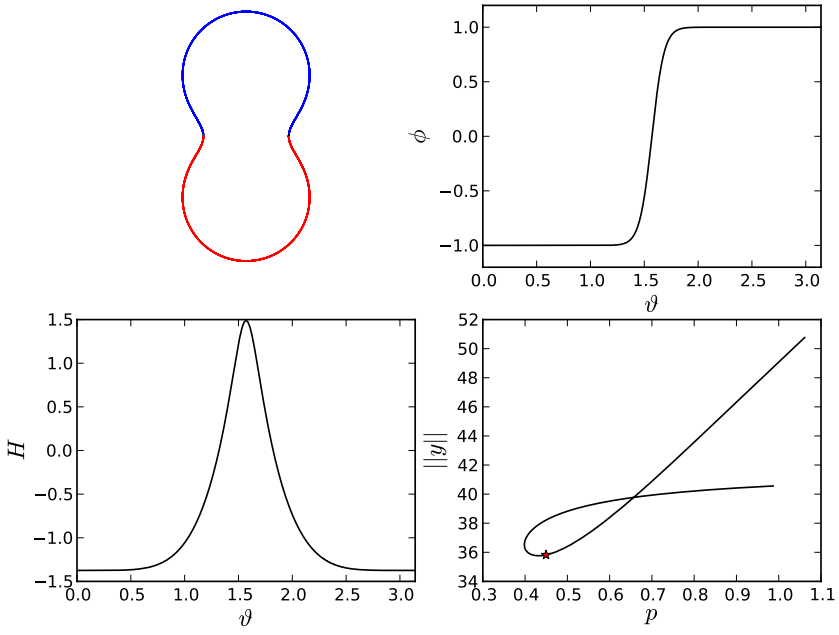


Figure 8.10: Symmetric First Mode for $p = 0.4496$

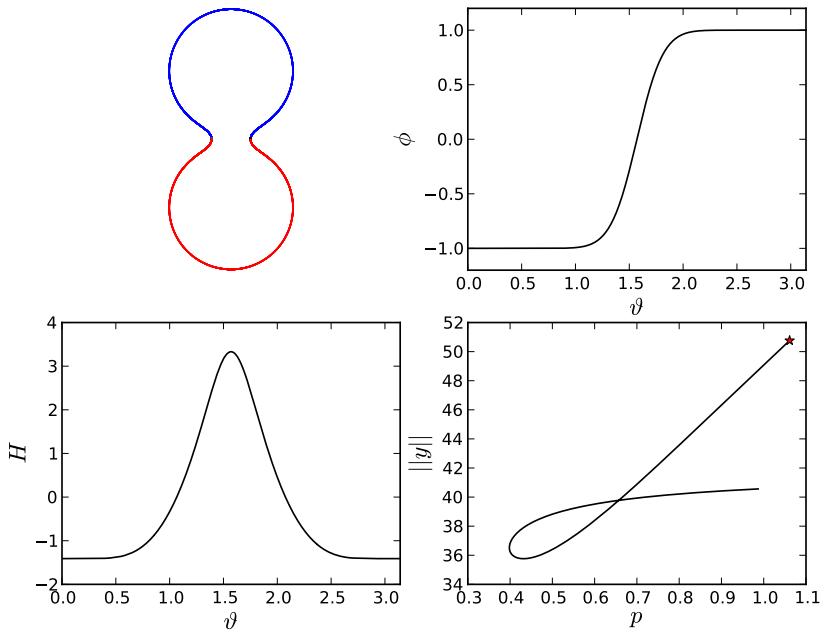


Figure 8.11: Symmetric First Mode for $p = 1.06123$

The presence of a limit point implies a possibility of change in stability. We now discuss the stability of the first mode. The first few eigen value of each block of the block-diagonalized hessian is separately computed using the Arnoldi scheme. The presence of a negative eigenvalue implies instability of the mode.

The following table gives the first five eigen values in the axisymmetric block of the hessian for solutions plotted in Figs. (8.8-8.11) as p is continued past the limit point

p=0.9867	p=0.4231	p=0.4496	p=1.06123
2.944627e-08	1.071625e-07	-3.606814e-01	-1.806864e+00
1.585552e+00	2.245185e-01	7.891838e-08	8.785372e-09
3.827317e+00	1.267597e+00	7.945587e-01	9.215616e-01
5.982601e+00	2.490499e+00	1.209844e+00	1.133157e+00
6.651736e+00	5.462420e+00	3.927318e+00	5.289393e+00

We observe that the lowest eigenvalue passes from a positive value to negative as we move past the limit point. The eigenvalue that is close to zero corresponds to the rigid translation mode in the z-direction. It is extremely important to note that the values in the table have been obtained when the constraint (4.23) for volume control is not enforced. Thus, we find that without volume control, the first mode losses stability as we move past the limit point to the more interesting pinched configurations.

The following table tabulates the (lowest five) eigen values of axisymmetric hessian block when the volume constraint is imposed. This is done by solving a constrained eigenvalue problem for the hessian using the linearized volume constraint, (4.24), using the method described in [29]. We find no negative eigen values as we pass through the limit point.

p=0.9867	p=0.4231	p=0.4496	p=1.06123
3.595904e-08	1.089508e-07	7.884817e-08	8.205802e-09
3.827317e+00	1.267597e+00	7.945587e-01	9.215616e-01
5.089031e+00	1.843428e+00	1.120394e+00	1.117741e+00
6.000116e+00	5.462420e+00	3.927318e+00	4.502715e+00
6.651736e+00	5.829448e+00	4.599849e+00	5.289393e+00

We now proceed to demonstrate that as we move past the limit point, the nonaxisymmetric blocks of the hessian do not loose stability when the volume control is imposed. This can be seen from the following two tables.

The first table below tabulates the lowest five eigen values for nonaxisymmetric blocks (labelled by the choice of m) for $p = 0.9867$, corresponding to figure (8.8) which is a representative solution point on one side of the limit point. The negative (near zero) eigenvalue in the $m = 1$ column can be safely neglected for stability as this corresponds to one of the rigid rotational mode. The lack of any negative eigenvalues in this table suggests that the corresponding solution is stable.

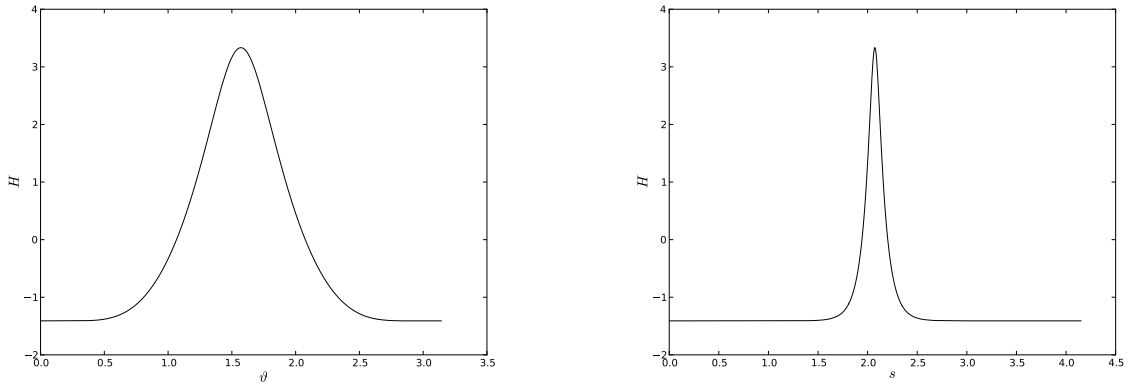
m=1	m=2	m=3	m=10	m=50
-6.005289e-07	2.360668e-02	6.105038e-02	7.256199e-01	1.814902e+01
1.253158e-09	2.479377e+00	5.990656e+00	6.723675e+00	2.413035e+01
1.617660e+00	4.712647e+00	6.696629e+00	8.781006e+00	2.633720e+01
4.648731e+00	6.018634e+00	8.083782e+00	8.914246e+00	2.685613e+01
6.035914e+00	8.041643e+00	8.134776e+00	9.068303e+00	2.744580e+01

In the second table, below, we tabulate the lowest five eigen values for nonaxisymmetric blocks (labelled by the choice m) for $p = 1.06123$ which corresponds to a solution on the other side of the limit point, shown on figure (8.11). Just like in the above case, the negative (near zero) eigenvalue in the $m = 1$ corresponds to a

rotational mode and can be be disregarded for stability. We see that this solution is also stable.

m=1	m=2	m=3	m=10	m=50
-9.861108e-09	6.510704e-01	1.284294e+00	9.356241e+00	3.944067e+01
2.867033e-08	3.304953e+00	5.875562e+00	9.356241e+00	3.944067e+01
2.904585e-01	3.332309e+00	8.147801e+00	9.627394e+00	4.069812e+01
4.705328e-01	3.762528e+00	8.148012e+00	9.627394e+00	4.069812e+01
3.642567e+00	8.072703e+00	8.245361e+00	9.923084e+00	4.198018e+01

Thus, we find that with volume control, the first symmetric mode is stable.



(a) Mean curvature as a function of ϑ (b) Mean curvature as a function of arc-length

Figure 8.12:

In figure (8.12(a)), we plot the mean curvature, H, as a function of ϑ, for the solution shown in figure (8.11). Notice that although the solution is itself highly pinched, the mean curvature is not sufficiently sharp. This should not be troubling because we are plotting H with respect to ϑ,a conformal coordinate, that is automatically being determined by the gauge equation. For comparison, we plot the mean curvature as a function of the arc-length in figure (8.12(b)). It is clear from this figure that H has a relatively steep peak, as we expected.

8.1.2 First Mode:Unsymmetric Case

Unsymmetrical vesicle shapes can be obtained by setting μ to a non-zero value. Recall that μ is the average value of ϕ on the surface of the vesicle. We follow a similar strategy to the previous symmetric case.

Figures (8.13) and (8.14) show shapes as ϵ is decreased while fixing the bending stiffness, $c = 1$, and pressure, $p = 1$. Once the vesicle is sufficiently phase separated, we fix ϵ at 0.0067 and c is decreased to 0.0012. Figures (8.15)-(8.17) show shapes corresponding to this decrease. Finally in figures (8.18)-(8.20) we fix ϵ at 0.0067 and c at 0.0012 and change the pressure. Similar to the symmetric case, a limit point is detected. The number of elements (N) in this case is chosen to be 200.

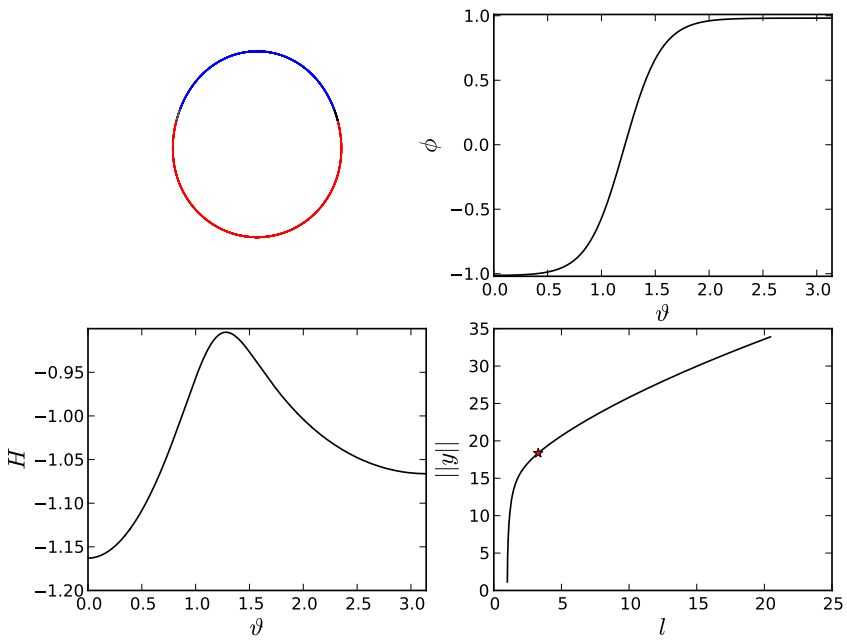


Figure 8.13: Unsymmetric First Mode for $\epsilon = 0.2078$

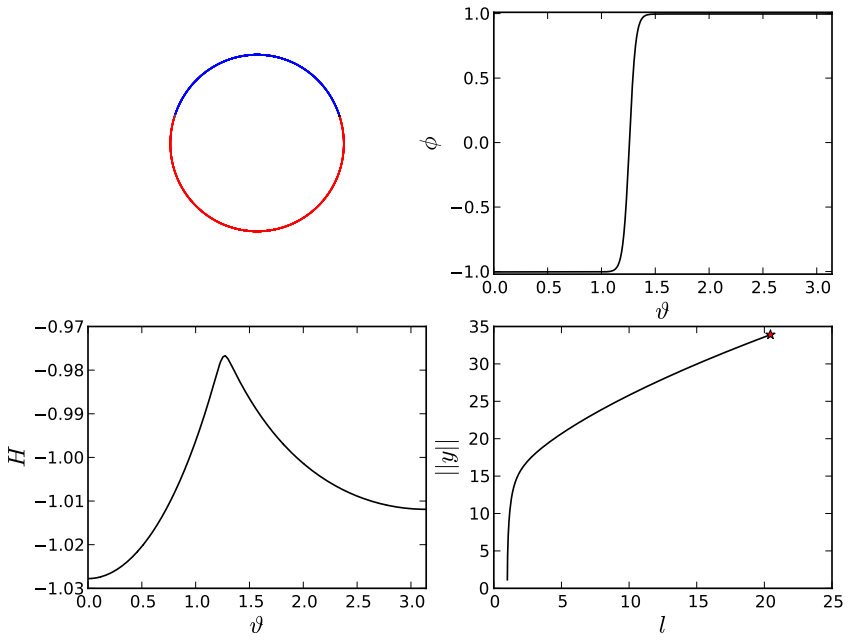


Figure 8.14: Unsymmetric First Mode for $\epsilon = 0.0067$

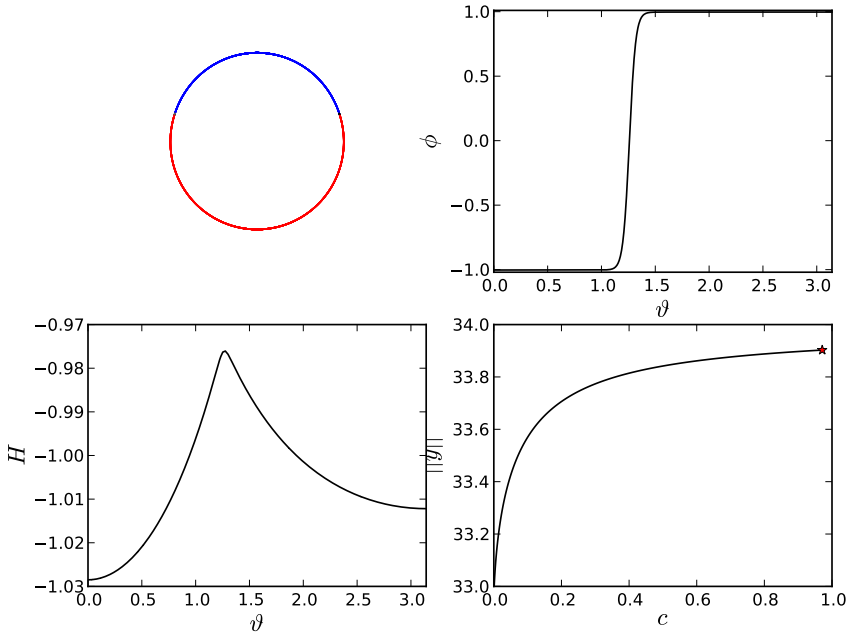


Figure 8.15: Unsymmetric First Mode for $c = 0.9711$

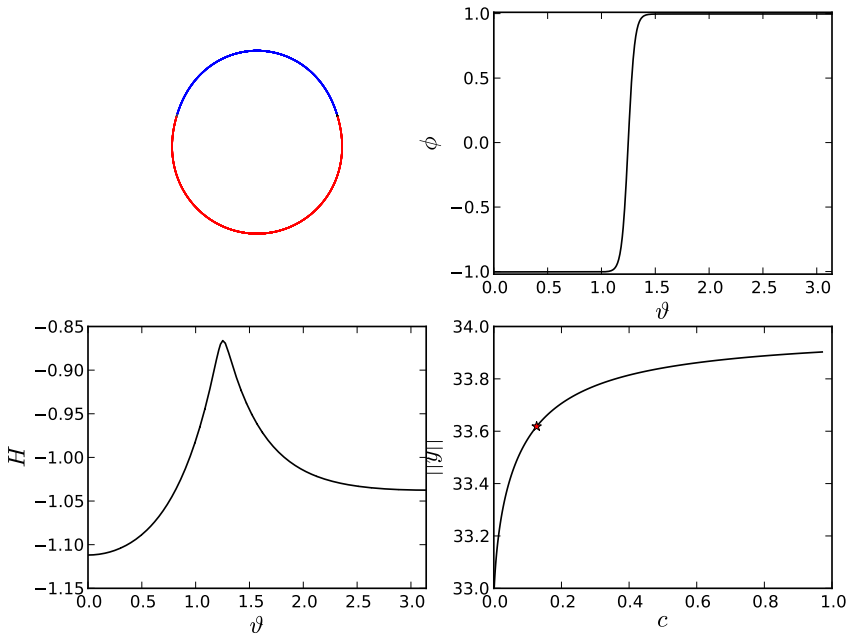


Figure 8.16: Unsymmetric First Mode for $c = 0.1266$

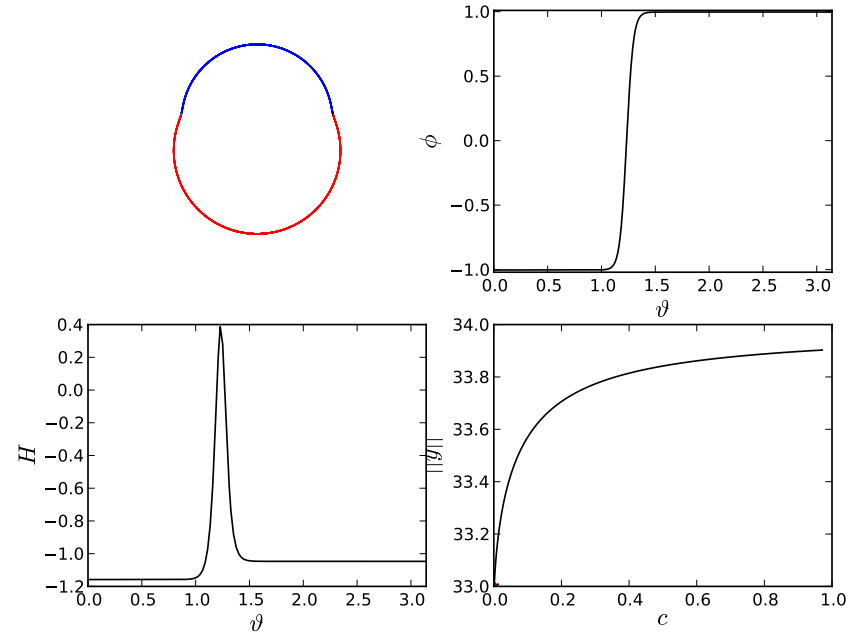


Figure 8.17: Unsymmetric First Mode for 0.0012

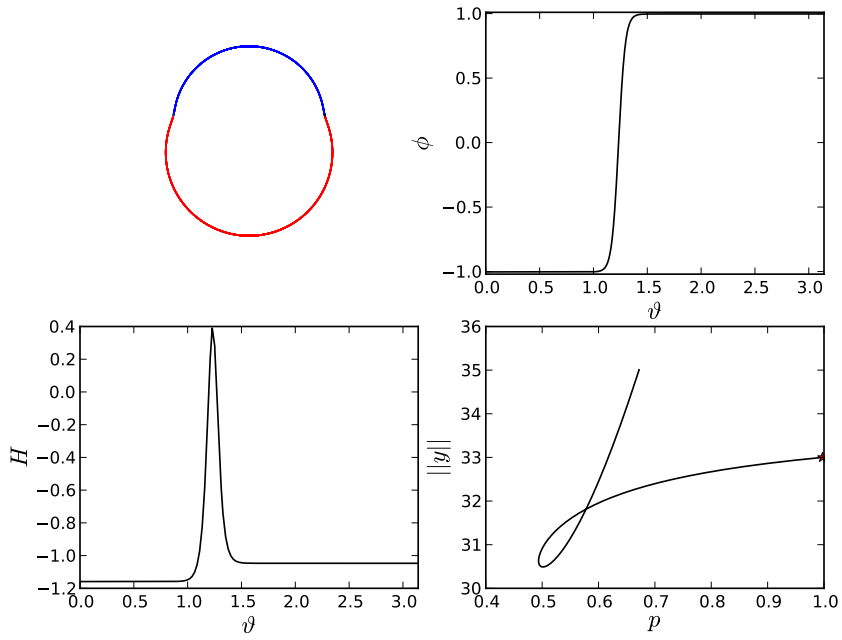


Figure 8.18: Unsymmetric First Mode for $p = 0.9972$

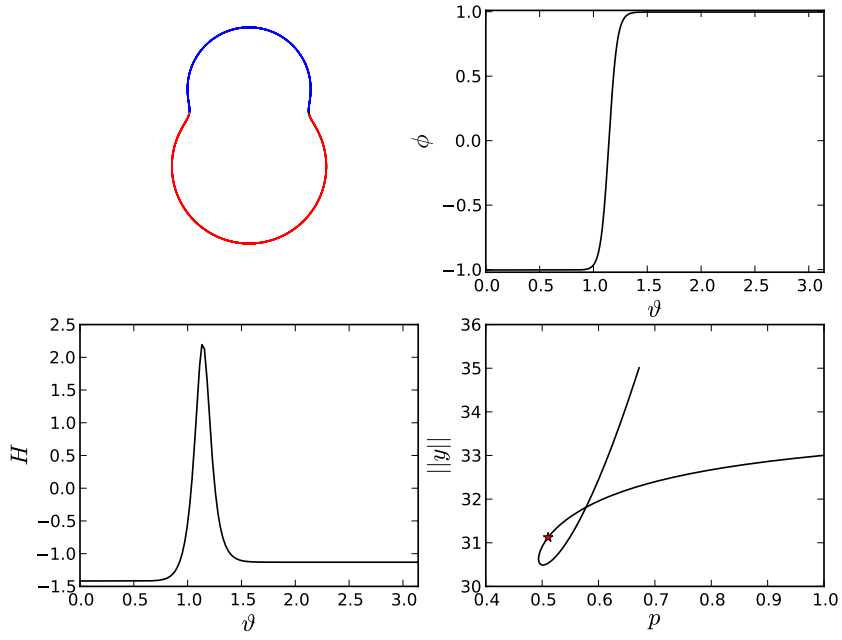


Figure 8.19: Unsymmetric First Mode for $p = 0.5105$

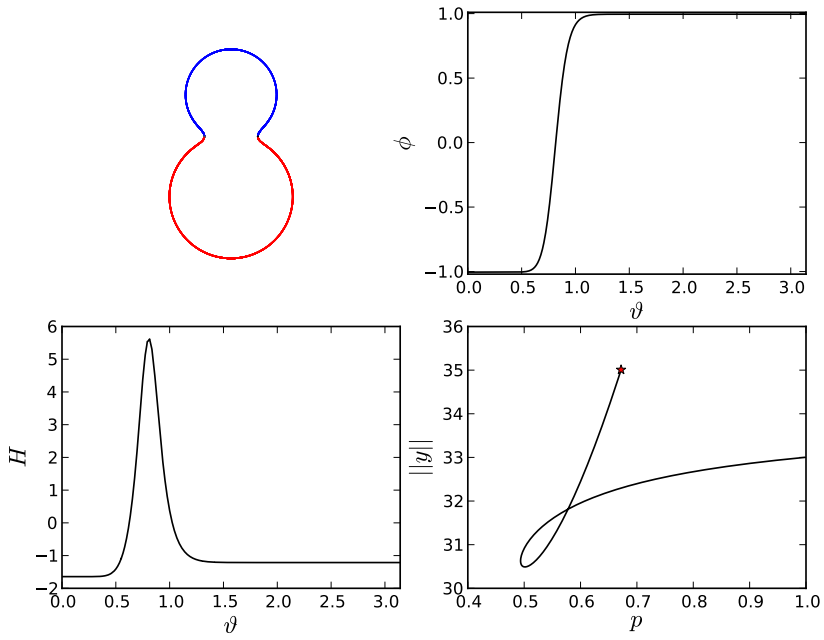


Figure 8.20: Unsymmetric First Mode for $p = 0.6719$

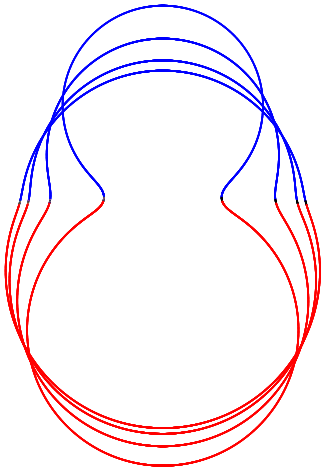


Figure 8.21: Unsymmetric vesicle pinches as we continue past the limit point.

We now discuss the stability of the unsymmetric mode. In the following table, the lowest five eigenvalues of the axisymmetric hessian block has been tabulated for two specific choices of pressure, p, which correspond to solutions on either side of the limit point seen in figure (8.20). In this case, the volume control is not imposed.

p=0.9972	p=0.6719
2.384570e-07	-3.118565e-01
1.272466e+00	1.226036e-06
3.778035e+00	6.964033e-01
5.768309e+00	1.207679e+00
6.395647e+00	3.208519e+00

Just like in the symmetric mode, we note the presence of a negative eigenvalue as we move past the limit point. This indicates a loss in stability past the limit point.

When the volume constraint is imposed, cf. (4.23), (4.24), all the eigenvalues (for the axisymmetic block) remain positive, as can be seen in the table below.

p=0.9972	p=0.6719
2.384762e-07	1.226011e-06
2.469432e+00	6.802000e-01
5.752366e+00	1.207635e+00
6.075448e+00	3.194515e+00
6.701189e+00	4.127853e+00

Eigenvalues for the nonaxisymmetric blocks are tabulated below. The value of pressure chosen in this case is $p = 0.6719$.

m=1	m=2	m=3	m=10	m=50
-1.093247e-06	2.674716e-01	5.542210e-01	5.170183e+00	3.286148e+01
3.929693e-06	1.388241e+00	2.846605e+00	8.967934e+00	3.386031e+01
2.480873e-01	1.737682e+00	4.244670e+00	9.183356e+00	3.487872e+01
4.114502e-01	2.495657e+00	6.122703e+00	9.418279e+00	3.591672e+01
2.132071e+00	4.460163e+00	7.830589e+00	9.672266e+00	3.697431e+01

We remark that the negative (near zero) eigenvalue in the $m = 1$ column can be neglected as it corresponds to a rigid rotational mode.

8.1.3 Second Mode

To get to a pinch configuration of the second mode as observed in experimental results (for instance, shown in figure (2.2)), we follow the continuation strategy described above. The results are plotted in figures (8.22)-(8.27). The number of elements, N, used in this case are 300.

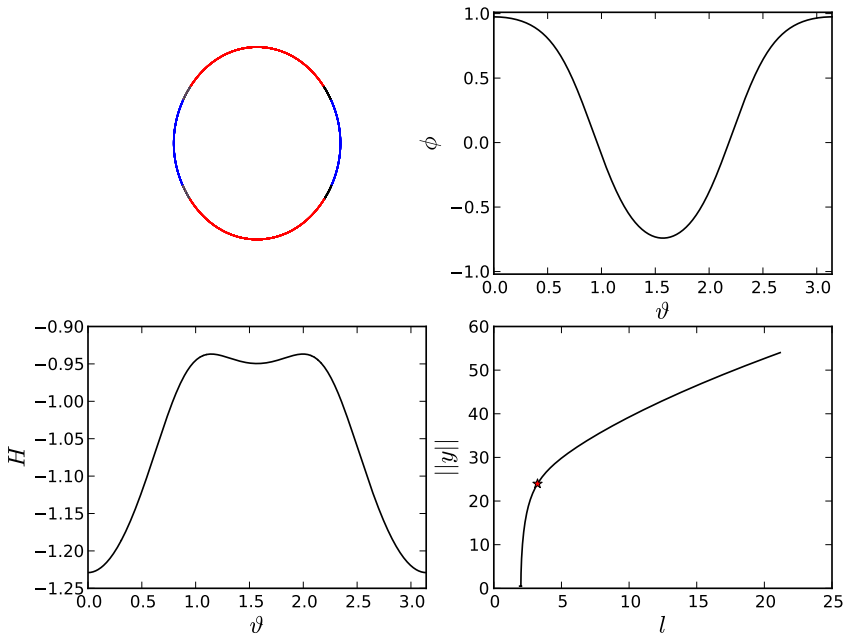


Figure 8.22: Second Mode for $\epsilon = 0.2927$

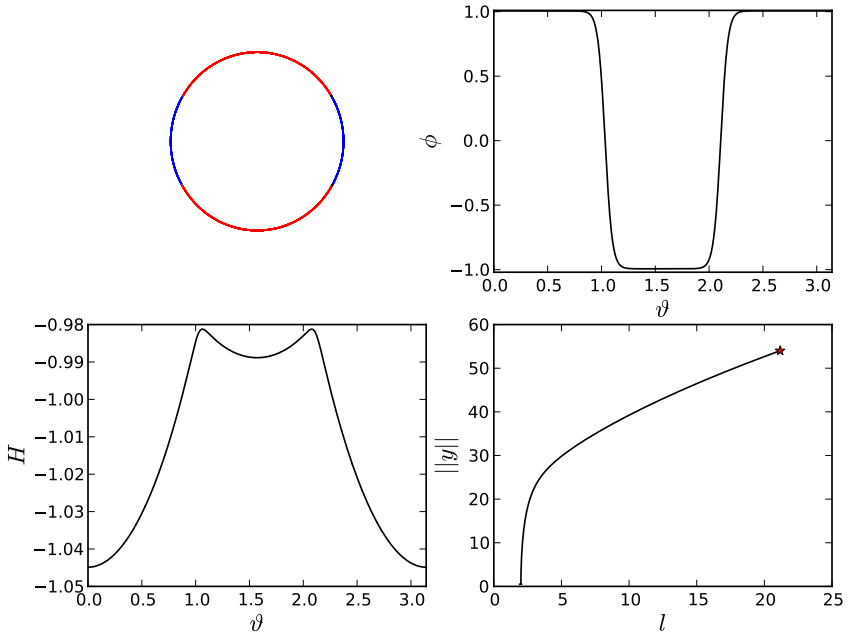


Figure 8.23: Second Mode for $\epsilon = 0.0085$

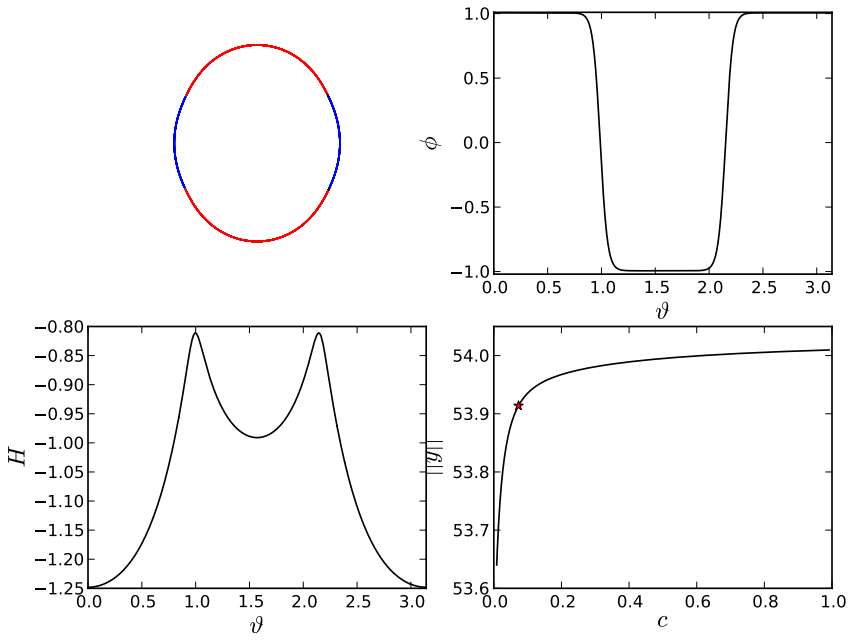


Figure 8.24: Second Mode for $c = 0.073$

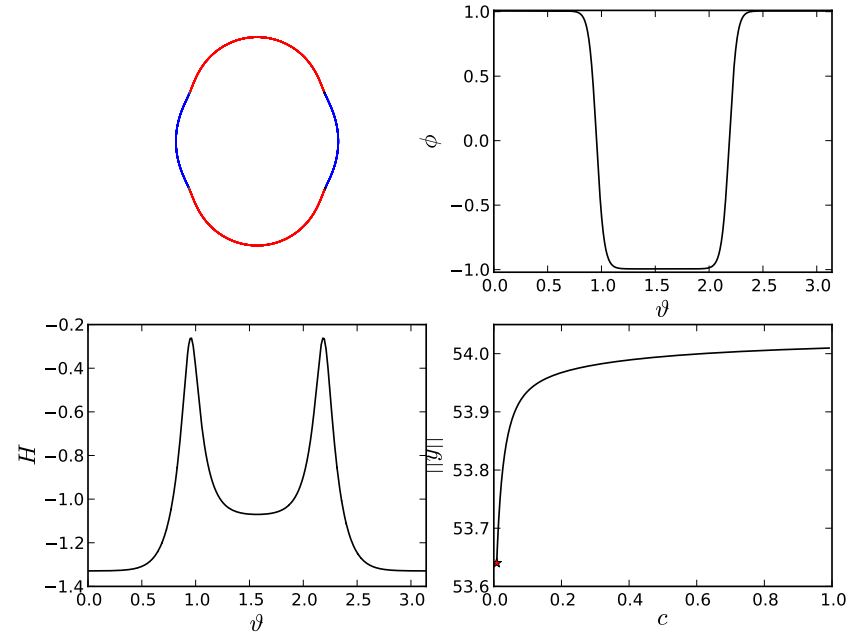


Figure 8.25: Second Mode for $c = 0.0085$

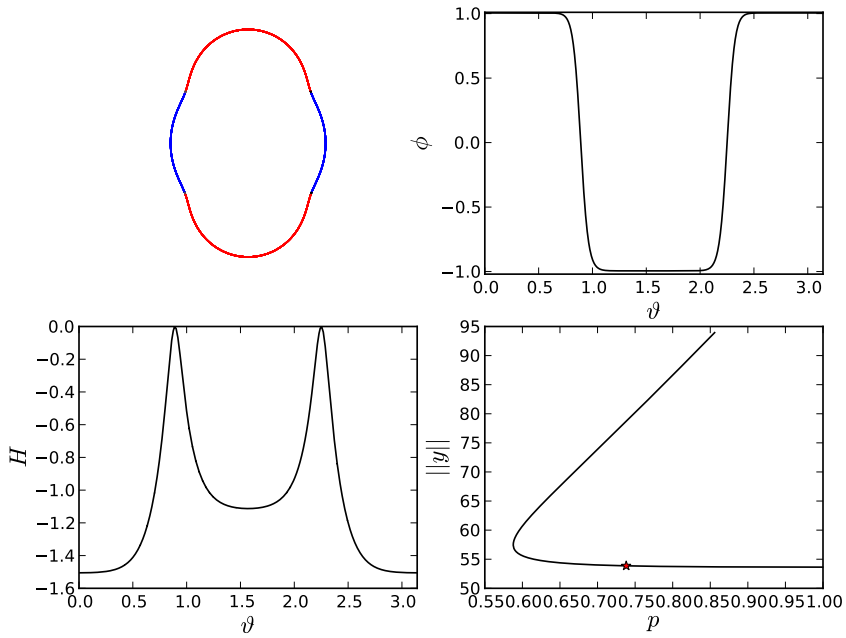


Figure 8.26: Second Mode for $p = 0.7381$

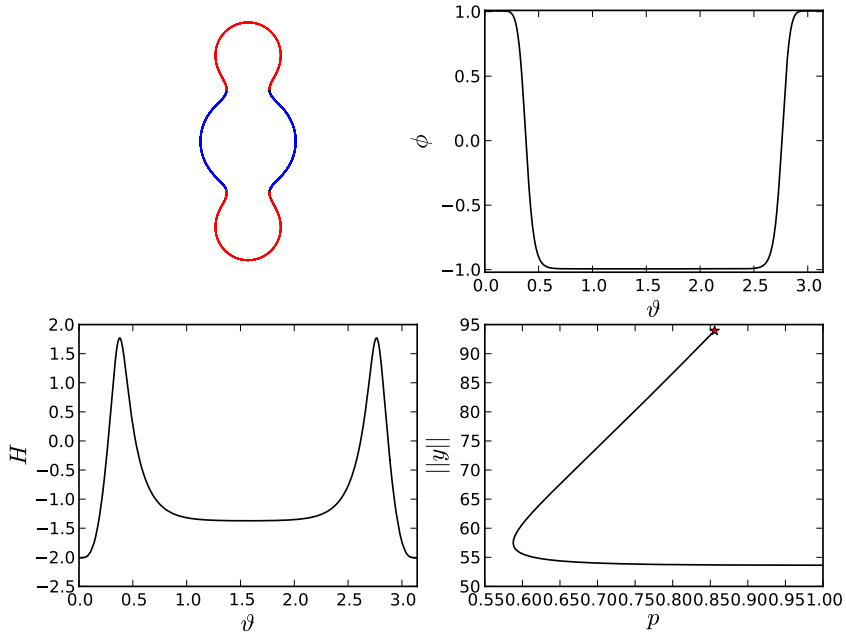
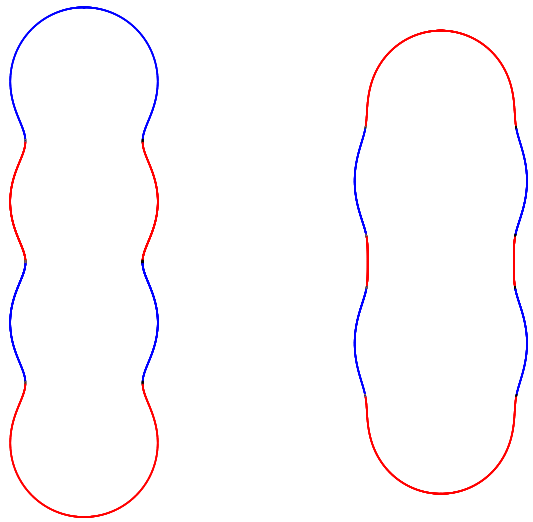


Figure 8.27: Second Mode for $p = 0.8558$

Stability analysis for this mode shows that there is always at least one negative eigenvalue in the axisymmetric block (with and without volume control). Thus, we find this mode to be unstable.

8.1.4 Third and Fourth Modes

By following the strategy described above, we obtain the the third and fourth modes shown in figure (8.28). Stability analysis of these modes (both with and without volume control) show them to be unstable.



(a) Third mode (b) Fourth mode

Figure 8.28:

8.1.5 Effect of Gaussian Bending Stiffness

So far, the gaussian bending stiffness, c_g, plays no role in our computations because by setting it to be independent of ϕ, it falls out of the Euler-Lagrange equations.

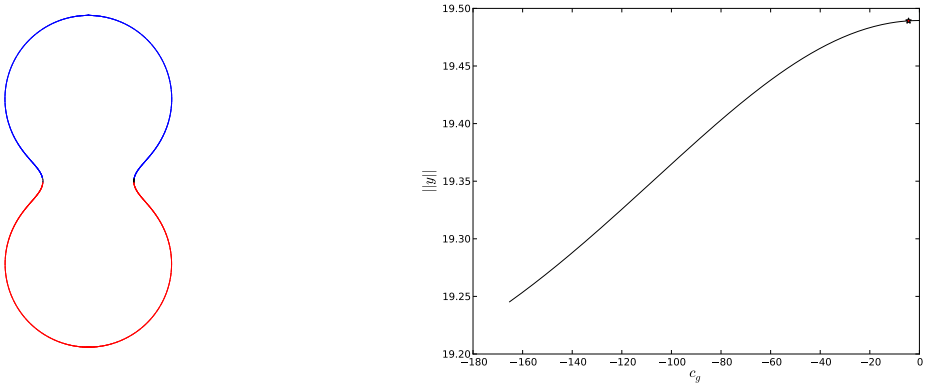


Figure 8.29: Relative difference in $c_g = -50\%$

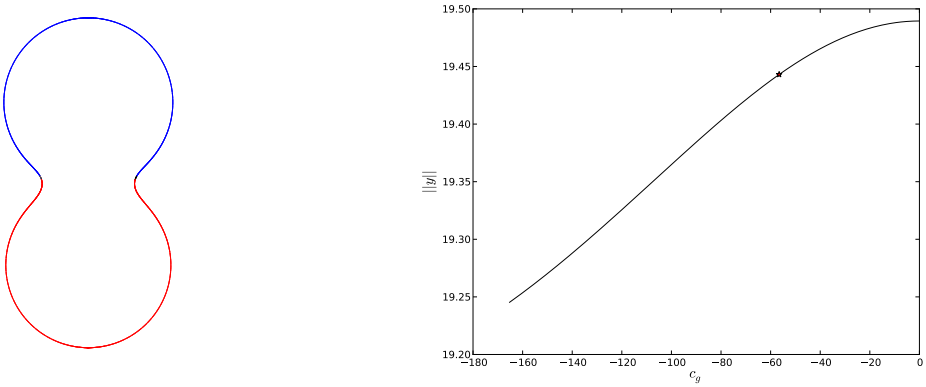


Figure 8.30: Relative difference in $c_g = -100\%$

We now treat the case when the gaussian bending stiffness depends on ϕ as shown in figure (2.3). The results for this case is shown in figures (8.29)-(8.32). We observe from these figures that the effect of change in the relative proportions of c_g is to move the position of the neck with respect to the phase boundary. This effect has been observed in the work of Das, *et. al.* [12].

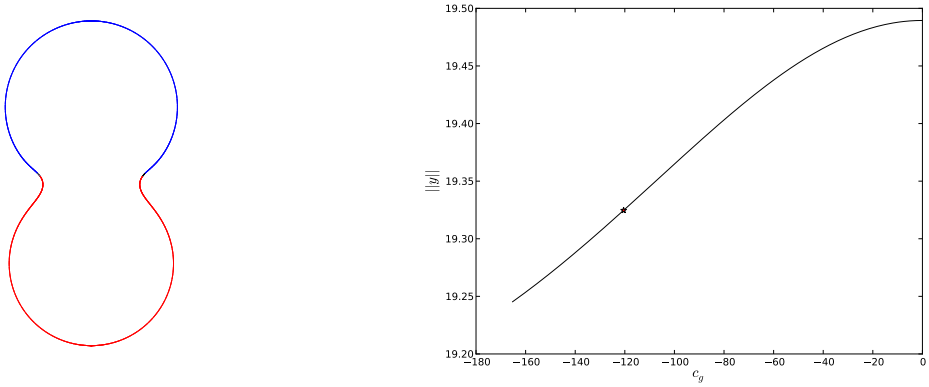


Figure 8.31: Relative difference in $c_g = -140\%$

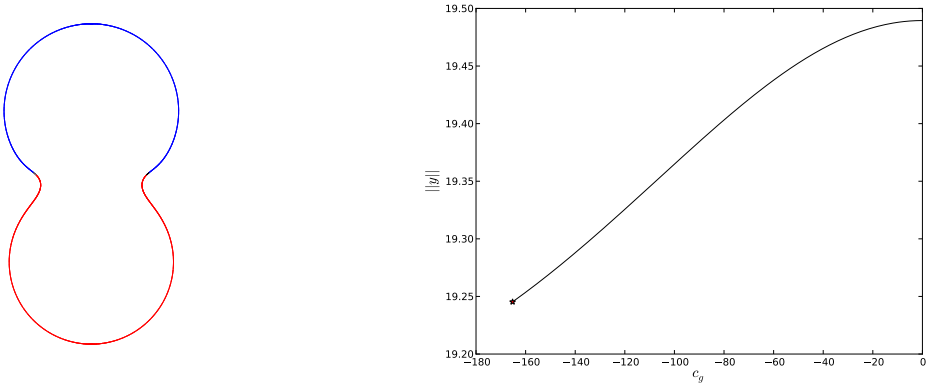


Figure 8.32: Relative difference in $c_g = -168\%$

CHAPTER 9

SUMMARY AND CONCLUSIONS

In this dissertation, a detailed and systematic study of phase transition in lipid bilayer membranes has been presented. The contributions of this work can be broadly categorized as theoretical and computational. We now summarize our essential finds and conclusions. Possible directions for future work are also indicated.

9.1 Summary

In chapter 2, the phenomenology of phase transitions in lipid membranes was presented and subsequently, a model that combined Cahn-Hilliard model with the Helfrich model was introduced. The ambiguity of choice between the local area constraint and the global area constraint was resolved by showing the two constraints to be equivalent for closed lipid membranes of genus zero. The Euler-Lagrange equations for the system was presented. The indeterminacy in the Euler-Lagrange equation and its relation to reparametrization invariance of the system via Nöther's second theorem was also discussed.

In chapter 3, the local bifurcation analysis was presented. Although standard tools from local bifurcation theory could not be directly applied because of the high dimensionality of the null space (of the linearization) the difficulty was circumvented by using group theoretic methods. A brief summary of such methods was also presented. Using such strategies we established the existence of local branches of solutions bifurcating from the trivial solution. We find these nontrivial solutions to lie in one-dimensional fixed point spaces of a specific symmetry subgroups of $O(3)$. These fixed point spaces are in fact symmetric spherical harmonics. The last section of the chapter was spent on summarizing Poole's procedure for explicitly constructing symmetric spherical harmonics based on Maxwell-Sylvester theorem.

Chapter 4 was concerned with the question of stability. The constraints involved in the formulation made the issue of stability a little delicate. Since stability depends on the nature of constraints imposed, we had to resolve the ambiguity of choice between a local area formulation and a global area formulation. Using tools from Hodge theory on Riemannian manifolds we showed that the two formulations could be treated to be equivalent for a genus zero lipid membranes. Volume constraint which was essential to stabilize solutions (as was seen in chapter 8) and its linearization was also discussed.

In chapter 5, we address the indeterminacy of the Euler-Lagrange equations and the existence of redundant degrees of freedom that can be ascribed to the reparametrization invariance of the system. We note the similarity of the lipid membrane system with other gauge theories of physics. In particular, the General theory of Relativity shares many features with our theory. For instance, the principle of covariance in GR is a reparametrization invariance of the theory. Inspired by GR we propose a gauge fixing procedure for the lipid membrane problem. The theory of *Harmonic maps* was introduced for this purpose. We showed, in the axisymmetric case, that by augmenting the Euler-Lagrange equations for the lipid membrane with the harmonic map equation (and certain other integral constraints) the gauge symmetry can be completely broken. The arguments for establishing this result used the equivalence of harmonic maps and conformal maps on genus zero surfaces. Riemann-Roch's theorem on the existence of conformal maps between genus zero surfaces guarantees that the gauge fixing procedure would always work. Apart from an intrinsic theoretical interest, the proposed gauge fixing procedure is tremendously useful for accurately computing solution branches. In particular, it avoids numerical issues such as mesh distortion that is frequently encountered in such problems in literature.

Chapters 6 and 7 were concerned with computational aspects of the problem. The discretization of the Euler-Lagrange equations was the focus of the former. After a brief review on numerical path following we presented the finite element formulation for the problem. The gauge equation, introduced in chapter 5 was augmented to the system of equilibrium equations and a weak formulation was derived. We concluded the chapter with a discussion on the discretization of the weak form using Galerkin projection. Throughout this work, computations are restricted to axisymmetric solutions.

Stability of the computed equilibria was the topic of interest in chapter 7. Although the solutions were axisymmetric, the importance of assembling the "full" hessian to determine stability was noted. However, a routine discretization of the hessian turned out to be computationally infeasible. An efficient way to discretize and assemble the hessian using symmetry adapted basis and block diagonalization technique was presented. Stability results in chapter 8 was obtained by using this technique where the individual hessian blocks were independently assembled and their eigenvalues was used to determine stability. A great advantage of this approach was the ability to avoid the assembly of the unnecessary zero entries of the hessian. This tremendously decreased the computational time and effort. Furthermore it may be noted that since the blocks could be assembled independently, parallelization is quite straightforward. The significant portion of the chapter was spent on using the projection operator theory to compute the symmetry adapted basis for the lipid membrane system. These calculations were restricted to the case where the underlying solution was axisymmetric.

Computational results of both equilibria and their stability were summarized in chapter 8. Axisymmetric solution paths were computed using path continuation on the discretized finite element system. The goal of the computation was to

systematically look for solutions similar to the ones observed in experiments and ascertain their stability. A strategy developed by Healey, *et al.* [31, 30] was used for this purpose. Solution paths for the first four modes were computed and their stability was determined by individually assembling the hessian blocks.

9.2 Conclusions

Our contributions in this work can be broadly categorized into theoretical and computational.

On the theoretical front, we have demonstrated the equivalence of formulations - LA and GA - based on local area and global area constraints, respectively. This equivalence is reflected not only in the Euler-Lagrange equations but also in stability. The techniques needed to show equivalence at the two levels were different.

It was seen in chapter 2 that the Euler-Lagrance equations for both the formulations were identical. However, that in itself is not sufficient to conclude that the formulations are equivalent. This is because the constraints imposed in the two formulations are different. Since local area preservation implies global area preservation, it is clear that solution set of the LA formulation is contained in the GA formulation. We show the converse by explicitly constructing a coordinate change which is used to reparametrize a solution that preserves area globally (GA) to a solution that preserves area locally. Reparametrization invariance of the GA formulation and the fact that the surface was of genus zero were crucial in the argument.

Although the expression for the second variation for both the LA and GA formulations are identical, the admissible class of variations for each of these formulations is different due to their differing constraints. To show equivalence, we had to show that the equivalence of the admissible class of variations. To be able

to do this on any arbitrary solution of the system, we relied on the Hodge decomposition theory on Riemannian manifolds. Zero genus of the surface was essential to show the equivalence.

Another theoretical contribution of this work was to address the indeterminacy in the Euler-Lagrange equations which is a manifestation of the reparametrization invariance of the system. For axisymmetric solutions, we did this by using the frame work of gauge theory and by proposing a gauge fixing procedure for the problem. This was done using the harmonic map equation. In fact, we showed that the harmonic map equation and certain other integral constraints to completely break the gauge symmetry of the problem. The case of non-axisymmetric solutions may be treated by supplementing the harmonic map equation with landmark constraints [24].

The third theoretical contribution was to (at least formally) establish local existence results for the problem. By using group theoretic strategies and choosing specific symmetry types for solutions, we were able to establish the existence of bifurcating branches from a spherical homogeneous trivial solution. Putting these arguments on a firm theoretical foundation will be the focus of our future work.

We have derived the second variation for the multiphase lipid bilayer problem about any arbitrary solution point. The advantage of having this expression is that we explicitly see that the tangential variations do not appear in the second variation. While computing stability, these tangential variations can be left out of the discretization and by doing their corresponding zero eigenvalues don't plague the numerics.

On the computational front, we have systematically computed axisymmetric solutions for the first four modes and their corresponding stability. We find that without imposing volume control, all the "interesting" solution branches (pinched

shapes observed in experiments) are unstable. With the volume control imposed, we find that the first mode is stabilized. However, volume control does not stabilize the higher modes. As the relative proportions of the gaussian stiffness moduli, c_g for each of the phases are changed, we find that the neck of the pinched shape moves relative to the phase boundary. This is consistent with observations made independently by other groups.

9.3 Future Work

There are several possible directions that can take based off the present work. Formal arguments for the local bifurcation analysis that were presented above could be made more rigorous. The challenge here is to find an appropriate framework to "mod out" the tangential displacements which always exist in the null space of the linearization. In our forthcoming paper [27], a symmetry-breaking global bifurcation analysis is presented, presuming a radial-graph placement field for the deformed surface. The case where global solutions cannot be captured by the radial-graph still remains to be explored.

A global bifurcation analysis of the problem is another exciting area worth exploring. The challenge here is formalizing the notion of solution, since solutions to the lipid membrane problem always exist in an equivalence class that is infinite dimension. The proposed gauge equation could find some good use in analysis, since it breaks the gauge symmetry to pick up a unique representative from the equivalence class.

Computationally there are lots of interesting possibilities. Systematic computation of nonaxisymmetric solutions and their stabilities has not yet been explored. Tracing secondary bifurcations is another rich and interesting area worth exploring.

APPENDIX A

VARIATION OF KINEMATIC QUANTITIES

In this chapter, we summarize the variations of the all important quantities that will be required to derive the first and second variations. Details of their derivation can be found in [57].

$$\delta g_{\alpha\beta} = \nabla_{(\alpha} v_{\beta)} - 2w b_{\alpha\beta}$$

$$\delta g^{\alpha\beta} = -\nabla^{(\alpha} v^{\beta)} + 2b^{\alpha\beta} w$$

$$\delta g = 2g\nabla \cdot \mathbf{v} - 4gHw$$

$$\delta b_{\alpha\beta} = (\nabla_\alpha v^\nu - w b^\nu_\alpha) b_{\nu\beta} + \nabla_\beta \left(v^\nu b_{\nu\alpha} + \nabla_\alpha w\right)$$

$$\delta H = (2H^2 - K)w + \frac{1}{2}\Delta w + \nabla H \cdot \mathbf{v}$$

$$\delta K = \tilde{\Delta} w + 2KHw + \nabla K \cdot \mathbf{v}$$

APPENDIX B

DERIVATION OF EULER-LAGRANGE EQUATIONS

To derive the Euler-Lagrange equations we take the first variation of the energy (2.8a) with respect to the unknowns $\mathbf{x} = \mathbf{f}(\mathbf{X})$ and $\phi(\mathbf{x})$. Recall that for sufficiently small α, we have the following variations,

$$\mathbf{x} \mapsto \mathbf{x} + \alpha[\mathbf{v} + w\mathbf{n}] =: \mathbf{x} + \alpha\delta\mathbf{x} \tag{B.1}$$

$$\phi(\mathbf{x}) \mapsto \phi(\mathbf{x}) + \alpha[\psi + \nabla\phi \cdot \mathbf{v}] =: \phi + \alpha\delta\phi \tag{B.2}$$

We obtain the Euler-Lagrange by setting the first variation of the energy to zero, i.e.,

$$\frac{d}{d\alpha}\mathcal{E}[\mathbf{x} + \alpha(\mathbf{v} + w\mathbf{n}), \phi + \alpha(\psi + \nabla\phi \cdot \mathbf{v})]|_{\alpha=0} = 0 \tag{B.3}$$

$$\begin{aligned}
\Rightarrow \int_\omega \left(2cH\delta H + c'H^2\delta\phi\right) + \left(c_g\delta K + c_g'K\delta\phi\right)\ da + \left(cH^2 + c_gK\right)\ \delta(da) + \\
\int_\omega \left(W'(\phi)\delta\phi + \frac{\epsilon}{2}(\phi_\alpha\phi_\beta\delta g^{\alpha\beta} + 2g^{\alpha\beta}\phi_\alpha(\delta\phi)_\beta)\right)\ da + \left(W + \frac{\epsilon}{2}|\nabla\phi|^2\right)\ \delta(da) + \\
\int_\omega (\gamma + \lambda(\phi - \mu))\ \delta(da) + \lambda\delta\phi\ da - p\delta V = 0.
\end{aligned}$$

Collecting like variations together,

$$\begin{aligned}
\int_\omega \left(2cH\delta H + c_g\delta K + \frac{\epsilon}{2}\phi_\alpha\phi_\beta\delta g^{\alpha\beta}\right)\ da + \left(cH^2 + c_gK + W + \right. \\
\left. \frac{\epsilon}{2}|\nabla\phi|^2 + \gamma + \lambda(\phi - \mu)\right)\ \delta(da) - p \\
\delta V + \int_\omega \left\{\left(W' + c'H^2 + c_g'K + \lambda\right)\delta\phi + \right. \\
\left. \epsilon g^{\alpha\beta}\phi_\alpha(\delta\phi)_\beta\right\}\ da.
\end{aligned}$$

Substituting the variations for various quantities involved, the first variation can be written as,

$$\int_\omega 2cH\Big\{(2H^2-K)w+\frac{1}{2}\Delta w+\mathbf{v}\cdot\nabla H\Big\}+\frac{\epsilon}{2}\nabla_\alpha\phi\nabla_\beta\phi\Big\{-\nabla^{(\alpha}v^{\beta)}+2b^{\alpha\beta}w\Big\}$$
$$c_g\Big(\tilde{\Delta}w+2KHw+\nabla K\cdot\mathbf{v}\Big)+$$
$$\Big(cH^2+c_gK+W+\frac{\epsilon}{2}|\nabla\phi|^2+\gamma+\lambda(\phi-\mu)\Big)\Big\{\nabla\cdot\mathbf{v}-2Hw\Big\}da-pw\;da$$
$$+\int_\omega \epsilon g^{\alpha\beta}\phi_\alpha(\delta\phi)_\beta+\Big(W'+c'H^2+c'_gK+\lambda\Big)\delta\phi\;da,$$

where $\tilde{\Delta}\cdot=\tilde{b}^{\alpha\beta}\nabla_\alpha\nabla_\beta$. We now integrate by parts to get,

$$\int_\omega\Big\{\tilde{\Delta}c_g+\Delta(cH)+2cH(H^2-K)+\epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta-2\tilde{\gamma}H-p\Big\}w+$$
$$\Big\{\epsilon\nabla\cdot(\nabla\phi\otimes\nabla\phi)-(c'H^2+c'_gK)\nabla\phi-\nabla\tilde{\gamma}\Big\}\cdot\mathbf{v}$$
$$\Big\{-\epsilon\Delta\phi+W'+\lambda+c'H^2+c'_gK\Big\}\delta\phi\;da,$$

where

$$\tilde{\gamma}=\frac{\epsilon}{2}|\nabla\phi|^2+W+\lambda(\phi-\mu)+\gamma \tag{B.4}$$

We replace the concentration variation, $\delta\phi$ using the following equation,

$$\delta\phi=\psi+\nabla\phi\cdot\mathbf{v},$$

to obtain,

$$\int_\omega\Big\{\tilde{\Delta}c_g+\Delta(cH)+2cH(H^2-K)+\epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta-2\tilde{\gamma}H-p\Big\}w+$$
$$\Big\{\epsilon\nabla\cdot(\nabla\phi\otimes\nabla\phi)-(c'H^2+c'_gK)\nabla\phi-\nabla\tilde{\gamma}\Big\}\cdot\mathbf{v}$$
$$\Big\{-\epsilon\Delta\phi+W'+\lambda+c'H^2+c'_gK\Big\}(\psi+\nabla\phi\cdot\mathbf{v})\;da.$$

Collecting all the independent variations together, we get,

$$\int_\omega \Big\{\tilde{\Delta} c_g + \Delta(cH) + 2cH(H^2 - K) + \epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta - 2\tilde{\gamma}H - p\Big\}w + \Big\{\epsilon\nabla\cdot(\nabla\phi\otimes\nabla\phi) - (\epsilon\Delta\phi - W' - \lambda)\nabla\phi - \nabla\tilde{\gamma}\Big\}\cdot\mathbf{v} \Big\{-\epsilon\Delta\phi + W' + \lambda + c'H^2 + c'_g K\Big\}\psi\, da.$$

APPENDIX C

SECOND VARIATION

C.1 Introduction

Consider the energy functional,

$$\mathcal{E} = \int_\omega c(\phi)H^2 + c_g(\phi)K + \gamma + \frac{1}{2}\epsilon|\nabla\phi|^2 + W(\phi) + \lambda(\phi-\mu)da - pV \tag{C.1}$$

Let $w, \mathbf{v}, \psi, \sigma, \tau$ represent variations in *normal,tangential*, ϕ, γ and λ, respectively. The first variation of the energy is:

$$\delta\mathcal{E} = \int_\omega \left[\mathcal{F}_n\delta\mathbf{r}\cdot\mathbf{n} + \mathcal{F}_\phi\psi\right]\, da + \int_\omega \sigma + \tau(\phi-\mu)\, da, \tag{C.2}$$

where,

$$\mathcal{F}_n := \epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta + \Delta(cH) + \tilde{\Delta}c_g + 2cH(H^2-K) - 2H\tilde{\gamma} - p, \tag{C.3}$$

$$\mathcal{F}_\phi := -\epsilon\Delta\phi + W' + \lambda + c'H^2 + c_g'K, \tag{C.4}$$

$$\tilde{\gamma} := \gamma + W + \frac{\epsilon}{2}|\nabla\phi|^2 + \lambda(\phi-\mu), \tag{C.5}$$

satisfying the following constraints,

$$\int_\omega da = 4\pi, \tag{C.6}$$

$$\int_\omega (\phi-\mu)\, da = 0. \tag{C.7}$$

With this proposition, the second variation of the energy can be written in the following way,

$$\delta^2\mathcal{E} = \int_\omega \delta\mathcal{F}_n w + \mathcal{F}_n(\delta\mathbf{r}\cdot\delta\mathbf{n}) + \delta\mathcal{F}_\phi\psi\, da + \int_\omega \underbrace{\left[\mathcal{F}_n w + \mathcal{F}_\phi\psi\right]}_{=0}\, \delta(da)$$
$$+ \int_\omega \tau(\psi + \nabla\phi\cdot\mathbf{v})\, da + \left[\sigma + \tau(\phi-\mu)\right]\delta(da).$$

By using the following definitions, $\hat{\mathcal{F}}_n := \delta\mathcal{F}_n$, $\hat{\mathcal{F}}_{\mathbf{t}} := \delta\mathcal{F}_{\mathbf{t}}$, $\hat{\mathcal{F}}_\phi := \delta\mathcal{F}_\phi$ to simplify our notation and using the fact that, at equilibrium $\mathcal{F}_\phi = 0$ and $\nabla\delta\gamma = 0$, we have,

$$\delta^2\mathcal{E} = \int_\omega \hat{\mathcal{F}}_n w + \hat{\mathcal{F}}_\phi \psi + \tau(\psi + \nabla\phi \cdot \mathbf{v})\, da + [\sigma + (\phi - \mu)\tau]\, \delta(da). \tag{C.8}$$

By observing that $\delta(da) = (\nabla \cdot \mathbf{v} - 2Hw)da$, we have,

$$\delta^2\mathcal{E} = \int_\omega \hat{\mathcal{F}}_n w + \hat{\mathcal{F}}_\phi \psi + \tau(\psi + \nabla\phi \cdot \mathbf{v})\, da + [\sigma + (\phi - \mu)\tau](\nabla \cdot \mathbf{v} - 2Hw)\, da. \tag{C.9}$$

It is important to note that the variations $\mathbf{v}$, w, ψ must respect the linearized constraints. That is,

$$\int_\omega (\nabla \cdot \mathbf{v} - 2Hw)\, da = 0, \tag{C.10}$$

$$\int_\omega [\psi + \nabla\phi \cdot \mathbf{v} + (\phi - \mu)(\nabla \cdot \mathbf{v} - 2Hw)]\, da = 0. \tag{C.11}$$

Using the above two conditions, we can further simplify the second variation as follows,

$$\delta^2\mathcal{E} = \int_\omega \hat{\mathcal{F}}_n w + \hat{\mathcal{F}}_\phi \psi\, da, \tag{C.12}$$

such that,

$$\int_\omega Hw\, da = 0, \tag{C.13}$$

$$\int_\omega (\psi - 2Hw\phi)\, da = 0. \tag{C.14}$$

where, we have obtained the above conditions by integrating the linearized constraint equations by parts.

C.2 Linearization of the Laplacian

Let $f : S^2 \to \mathbb{R}$ be any scalar field on the sphere. The Laplacian of f with respect to the metric $g^{\alpha\beta}$ is given by,

$$\Delta f = \frac{1}{\sqrt{g}}\partial_\alpha[\sqrt{g}g^{\alpha\beta}\partial_\beta f].$$

Variation in the surface induces the following variations,

$$g \mapsto g + \xi\mathfrak{g},$$

$$g^{\alpha\beta} \mapsto g^{\alpha\beta} + \xi\mathfrak{g}^{\alpha\beta},$$

$$\Delta \mapsto \Delta + \xi\mathcal{L}.$$

The following two lemmas are immediate.

Lemma 5. *For any scalar function f,*

$$\delta(\Delta f) = \Delta(\delta f) + \mathcal{L}f.$$

Lemma 6.

$$\delta(\Delta\phi) = \Delta(\psi + \mathbf{v}\cdot\nabla\phi) + \mathcal{L}\phi.$$

Proposition 9.

$$\mathcal{L}f = \nabla_\alpha[\mathfrak{g}^{\alpha\beta}\nabla_\beta f] + \nabla^\alpha f\nabla_\alpha(\frac{\mathfrak{g}}{2g})$$

Proof. Since $g \mapsto g + \xi\mathfrak{g}$, we have, $\sqrt{g} \mapsto \sqrt{g}(1 + \xi\frac{\mathfrak{g}}{2g})$, $1/\sqrt{g} \mapsto \frac{1}{\sqrt{g}}(1 - \xi\frac{\mathfrak{g}}{2g})$

$$\Delta\cdot \mapsto \frac{1}{\sqrt{g}}(1 - \frac{\mathfrak{g}}{2g}\xi)\partial_\alpha[\sqrt{g}(1 + \frac{\mathfrak{g}}{2g}\xi)(g^{\alpha\beta} + \xi\mathfrak{g}^{\alpha\beta})\partial_\beta\cdot]$$

$$= \frac{1}{\sqrt{g}}(1 - \frac{\mathfrak{g}}{2g}\xi)\partial_\alpha[\sqrt{g}g^{\alpha\beta}\partial_\beta + \xi\sqrt{g}(\mathfrak{g}^{\alpha\beta}\cdot + \frac{\mathfrak{g}}{2g}g^{\alpha\beta})\partial_\beta\cdot] + \cdots$$

$$= \frac{1}{\sqrt{g}}\partial_\alpha(\sqrt{g}g^{\alpha\beta}\partial_\beta\cdot) + \xi\left\{\frac{1}{\sqrt{g}}\partial_\alpha[\sqrt{g}(\mathfrak{g}^{\alpha\beta} + \frac{\mathfrak{g}}{2g}g^{\alpha\beta})\partial_\beta\cdot] - \frac{\mathfrak{g}}{2g\sqrt{g}}\partial_\alpha(\sqrt{g}g^{\alpha\beta}\partial_\beta)\right\} + \cdots$$

$$= \Delta\cdot + \xi\left\{\frac{1}{\sqrt{g}}\partial_\alpha(\sqrt{g}\mathfrak{g}^{\alpha\beta}\partial_\beta\cdot) + \frac{1}{\sqrt{g}}\partial_\alpha(\sqrt{g}\frac{\mathfrak{g}}{2g}g^{\alpha\beta}\partial_\beta\cdot) - \frac{\mathfrak{g}}{2g\sqrt{g}}\partial_\alpha(\sqrt{g}g^{\alpha\beta}\partial_\beta\cdot)\right\} + \cdots$$

$$= \Delta\cdot + \xi\left\{\frac{1}{\sqrt{g}}\partial_\alpha(\sqrt{g}\mathfrak{g}^{\alpha\beta}\partial_\beta\cdot) + \frac{1}{\sqrt{g}}\partial_\alpha(\frac{\mathfrak{g}}{2g})\sqrt{g}g^{\alpha\beta}\partial_\beta\cdot\right\} + \cdots$$

Therefore,

$$\mathcal{L}\cdot = \nabla_\alpha(\mathfrak{g}^{\alpha\beta}\nabla_\beta f) + \nabla^\alpha f \nabla_\alpha(\frac{\mathfrak{g}}{2g})$$

. □

Proposition 10.

$$\mathcal{L}f = \mathcal{L}^{(n)}f + \mathcal{L}^{(\mathbf{t})}f,$$

where,

$$\mathcal{L}^{(n)}f = 2[\nabla_\alpha(b^{\alpha\beta}w\nabla_\beta f) - \nabla_\alpha(Hw)\nabla^\alpha f],$$

$$\mathcal{L}^{(\mathbf{t})}f = -[\Delta v^\beta \nabla_\beta f + Kv^\beta\nabla_\beta f + 2\nabla^\alpha v^\beta \nabla_\alpha\nabla_\beta f].$$

Proof. Recall the following,

$$\mathfrak{g}^{\alpha\beta} = -\nabla^{(\alpha}v^{\beta)} + 2b^{\alpha\beta}w,$$

$$\frac{\mathfrak{g}}{2g} = \nabla_\alpha v^\alpha - 2Hw,$$

By the proposition (9),

$$\mathcal{L}f = \nabla_\alpha(\mathfrak{g}^{\alpha\beta}\nabla_\beta f) + \nabla^\alpha f\nabla_\alpha(\frac{\mathfrak{g}}{2g})$$

$$= \nabla_\alpha\left\{2b^{\alpha\beta}w\nabla_\beta f - \nabla^{(\alpha}v^{\beta)}\nabla_\beta f\right\} + \nabla^\alpha f\nabla_\alpha[\nabla_\gamma v^\gamma - 2Hw]$$

$$= 2\left\{\nabla_\alpha(b^{\alpha\beta}w\nabla_\beta f) - \nabla_\alpha(Hw)\nabla^\alpha f\right\} - \nabla_\alpha(\nabla^{(\alpha}v^{\beta)}\nabla_\beta f) + \nabla^\alpha f\nabla_\alpha\nabla_\gamma v^\gamma$$

$$= \mathcal{L}^{(n)}f - \nabla_\alpha(\nabla^{(\alpha}v^{\beta)})\nabla_\beta f - \nabla^{(\alpha}v^{\beta)}\nabla_\alpha\nabla_\beta f + \nabla^\alpha f\nabla_\alpha\nabla_\gamma v^\gamma.$$

Observe that $\nabla_\alpha\nabla_\beta f = \nabla_\beta\nabla_\alpha f$, that is, the second derivatives of a scalar field commute and thus is symmetric. By relabling indices in this term, we get

$$\mathcal{L}f = \mathcal{L}^{(n)}f - \nabla_\alpha(\nabla^{(\alpha}v^{\beta)})\nabla_\beta f - 2\nabla^\alpha v^\beta\nabla_{\alpha\beta}f + \nabla^\alpha f\nabla_\alpha\nabla_\gamma v^\gamma$$

$$= \mathcal{L}^{(n)}f - \nabla_\alpha(\nabla^\alpha v^\beta + \nabla^\beta v^\alpha)\nabla_\beta f - 2(\nabla^\alpha v^\beta)\nabla_{\alpha\beta}f + \nabla^\alpha f\nabla_\alpha\nabla_\gamma v^\gamma$$

$$= \mathcal{L}^{(n)} f - \Delta v^\beta \nabla_\beta f - 2\nabla^\alpha v^\beta \nabla_{\alpha\beta} f - \nabla^\beta f [\nabla_\alpha \nabla_\beta - \nabla_\beta \nabla_\alpha] v^\alpha.$$

Recall the following facts,

$$[\nabla_\alpha \nabla_\beta - \nabla_\beta \nabla_\alpha] v^\gamma = \mathcal{R}^\gamma_{.\delta\alpha\beta} v^\delta,$$

$$\mathcal{R}^\alpha_{.\delta\alpha\beta} = K g_{\delta\beta}.$$

So, we have,

$$[\nabla_\alpha \nabla_\beta - \nabla_\beta \nabla_\alpha] v^\alpha = K g_{\delta\beta} v^\delta.$$

Hence,

$$\mathcal{L} f = \mathcal{L}^{(n)} f - \Delta v^\alpha \nabla_\alpha f - 2\nabla^\alpha v^\beta \nabla_{\alpha\beta} f - K \nabla_\beta f v^\beta.$$

□

Proposition 11. *For any scalar field f,*

$$\Delta \nabla_\alpha f = \nabla_\alpha (\Delta f) + K \nabla_\alpha f$$

Proof.

$$\Delta \nabla_\alpha f = \nabla^\beta \nabla_\beta (\nabla_\alpha f) = \nabla^\beta (\nabla_\beta \nabla_\alpha f) = \nabla^\beta (\nabla_{\beta\alpha} f) = \nabla^\beta (\nabla_{\alpha\beta} f)$$

$$= \nabla_\beta \nabla_\alpha (\nabla^\beta f) = \nabla_\alpha \nabla_\beta (\nabla^\beta f) - \mathcal{R}^\beta_{.\delta\alpha\beta} \nabla^\delta f$$

$$= \nabla_\alpha \nabla_\beta (\nabla^\beta f) + \mathcal{R}^\beta_{.\delta\beta\alpha} \nabla^\delta f$$

$$= \nabla_\alpha (\Delta f) + K g_{\alpha\delta} \nabla^\delta f.$$

□

C.3 Linearizing $\tilde{\Delta}$

Recall that $\tilde{\Delta}\cdot = \tilde{b}^{\alpha\beta}\nabla_\alpha\nabla_\beta\cdot$, where $\tilde{b}^{\alpha\beta}$ is the cofactor of the curvature tensor. Also, recall the fact that the cofactor matrix is divergence-free, i.e., $\nabla_\alpha\tilde{b}^{\alpha\beta} = 0$. By Cayley-Hamilton, we have, $\tilde{b}^{\alpha\beta} = 2Hg^{\alpha\beta} - b^{\alpha\beta}$.

Proposition 12.

$$\mathfrak{b}^{\alpha\beta(\mathbf{t})} = -b^{\mu(\alpha}\nabla_\mu v^{\beta)} + v^\mu\nabla_\mu b^{\alpha\beta},$$

$$\mathfrak{b}^{\alpha\beta(n)} = 3b^{\alpha\mu}b^\beta_\mu + \nabla^{\alpha\beta}w.$$

Proof.

$$b^{\alpha\beta} = g^{\alpha\mu}g^{\beta\nu}b_{\mu\nu} \Rightarrow \mathfrak{b}^{\alpha\beta} = \mathfrak{g}^{\alpha\mu}b^\beta_\mu + \mathfrak{g}^{\beta\nu}b^\alpha_\nu + g^{\alpha\mu}g^{\beta\nu}\mathfrak{b}_{\mu\nu}$$

$$\mathfrak{b}^{\alpha\beta(\mathbf{t})} = -b^\beta_\mu\nabla^{(\alpha}v^{\mu)} - b^\alpha_\nu\nabla^{(\beta}v^{\nu)} + g^{\alpha\mu}g^{\beta\nu}[\nabla_\mu v^\sigma b_{\sigma\nu} + \nabla_\nu(v^\sigma b_{\sigma\mu})]$$

$$= -b^\beta_\mu\nabla^{(\alpha}v^{\mu)} - b^\alpha_\nu\nabla^{(\beta}v^{\nu)} + [\nabla^\alpha v^\sigma b^\beta_\sigma + \nabla^\beta(v^\sigma b^\alpha_\sigma)]$$

$$\mathfrak{b}^{\alpha\beta(w)} = (2b^{\alpha\mu}w)b^\beta_\mu + (2b^{\beta\mu}w)b^\alpha_\mu + g^{\alpha\mu}g^{\beta\nu}[-wb^\gamma_\mu b_{\gamma\nu} + \nabla_{\mu\nu}w]$$

$$= 4b^{\alpha\mu}b^\beta_\mu w - b^{\alpha\gamma}b^\beta_\gamma w + \nabla^{\alpha\beta}w$$

$$= 3b^{\alpha\mu}b^\beta_\mu + \nabla^{\alpha\beta}w.$$

□

Proposition 13.

$$\tilde{\mathfrak{b}}^{\alpha\beta(\mathbf{t})} = -\tilde{b}^{\mu(\alpha}\nabla_\mu v^{\beta)} + v^\mu\nabla_\mu\tilde{b}^{\alpha\beta},$$

$$\tilde{\mathfrak{b}}^{\alpha\beta(n)} = g^{\alpha\beta}\Delta w + 2H\tilde{b}^{\alpha\beta}w - \nabla^{\alpha\beta}w.$$

Proof.

$$\tilde{b}^{\alpha\beta} = 2Hg^{\alpha\beta} - b^{\alpha\beta} \Rightarrow \tilde{\mathfrak{b}}^{\alpha\beta} = 2\delta Hg^{\alpha\beta} + 2H\mathfrak{g}^{\alpha\beta} - \mathfrak{b}^{\alpha\beta}$$

$$\Rightarrow \tilde{\mathfrak{b}}^{\alpha\beta(\mathbf{t})} = 2g^{\alpha\beta}\delta^{(\mathbf{t})}H + 2H\mathfrak{g}^{\alpha\beta(\mathbf{t})} - \mathfrak{b}^{\alpha\beta(\mathbf{t})}$$

$$= 2v^\mu \nabla_\mu H g^{\alpha\beta} - 2H\nabla^{(\alpha} v^{\beta)} + b^{\mu(\alpha}\nabla_\mu v^{\beta)} - v^\mu \nabla_\mu b^{\alpha\beta}$$

$$= 2v^\mu \nabla_\mu H g^{\alpha\beta} - 2H\nabla^{\alpha} v^{\beta} - 2H\nabla^{\beta} v^{\alpha} + b^{\mu\alpha}\nabla_\mu v^{\beta} + b^{\mu\beta}\nabla_\mu v^{\alpha} - v^\mu \nabla_\mu b^{\alpha\beta}$$

$$= -\nabla_\mu v^\beta [2Hg^{\mu\alpha} - b^{\mu\alpha}] - \nabla_\mu v^\alpha [2Hg^{\mu\beta} - b^{\mu\beta}] + v^\mu \nabla_\mu \tilde{b}^{\alpha\beta}$$

$$= -\tilde{b}^{\mu(\alpha}\nabla_\mu v^{\beta)} + v^\mu \nabla_\mu \tilde{b}^{\alpha\beta}.$$

$$\tilde{\mathfrak{b}}^{\alpha\beta(n)} = 2g^{\alpha\beta}\delta^{(n)}H + 2H\mathfrak{g}^{\alpha\beta(n)} - \mathfrak{b}^{\alpha\beta(n)}$$

$$= 2\Big[\frac{\Delta w}{2} + (2H^2 - K)w\Big]g^{\alpha\beta} + 2H\Big[2b^{\alpha\beta}w\Big] - \Big[3b^{\alpha\mu}b^{\beta\mu}w + \nabla^{\alpha\beta}w\Big]$$

$$= g^{\alpha\beta}\Big[\Delta w + (4H^2 - 2K)w\Big] + \Big[4Hb^{\alpha\beta} - 3b^{\alpha\mu}b^{\beta}_{\mu}\Big] - \nabla^{\alpha\beta}w. \tag{C.15}$$

By Cayley-Hamilton, we have

$$b^{\alpha\mu}b^{\beta}_{\mu} - 2Hb^{\alpha\beta} + Kg^{\alpha\beta} = 0,$$

$$\Rightarrow b^{\alpha\mu}b^{\beta}_{\mu} = 2Hb^{\alpha\beta} - Kg^{\alpha\beta},$$

$$\Rightarrow -3b^{\alpha\mu}b^{\beta}_{\mu} = -6Hb^{\alpha\beta} + 2Kg^{\alpha\beta},$$

$$\Rightarrow (4Hb^{\alpha\beta} - 3b^{\alpha\mu}b^{\beta}_{\mu}) = -2Hb^{\alpha\beta} + 2Kg^{\alpha\beta}.$$

Using the above relation in equation (C.15), we have

$$\tilde{\mathfrak{b}}^{\alpha\beta(n)} = g^{\alpha\beta}\Delta w + (4H^2 - 2K)wg^{\alpha\beta} + \Big[-2Hb^{\alpha\beta}w + 2Kg^{\alpha\beta}w\Big] - \nabla^{\alpha\beta}w$$

$$= g^{\alpha\beta}\Delta w + 2H\Big(2Hg^{\alpha\beta} - b^{\alpha\beta}\Big)w - \nabla^{\alpha\beta}w$$

$$= g^{\alpha\beta}\Delta w + 2H\tilde{b}^{\alpha\beta}w - \nabla^{\alpha\beta}w.$$

□

Definition 23. *$\tilde{\mathcal{L}}\cdot$ is defined to be the linearization of the operator $\tilde{\Delta}\cdot$.*

Lemma 7.

$$\tilde{\mathcal{L}}f = \nabla_\alpha[\tilde{\mathfrak{b}}^{\alpha\beta}\nabla_\beta f] + \tilde{b}^{\alpha\beta}(\nabla_\beta f)\nabla_\alpha\left(\frac{\mathfrak{g}}{2g}\right).$$

Proof. Similar to the proof for $\mathcal{L}f$. □

Lemma 8.

$$\tilde{\mathcal{L}}^{(\mathbf{t})} f = -\tilde{\Delta}(\nabla f \cdot \mathbf{v}) + \mathbf{v} \cdot \nabla \tilde{\Delta} f.$$

Proof.

$$\tilde{\mathcal{L}}^{(\mathbf{t})} f = \nabla_\alpha [\tilde{\mathfrak{b}}^{\alpha\beta(\mathbf{t})} \nabla_\beta f] + \tilde{b}^{\alpha\beta} (\nabla_\beta f) \nabla_\alpha \left(\frac{\mathfrak{g}^{(\mathbf{t})}}{2g} \right)$$

$$= \nabla_\alpha [\tilde{\mathfrak{b}}^{\alpha\beta(\mathbf{t})} f_\beta] + \tilde{b}^{\alpha\beta} f_\beta \nabla_\alpha \nabla_\mu v^\mu$$

Substituting for $\tilde{\mathfrak{b}}^{\alpha\beta(\mathbf{t})}$ using proposition (13),

$$\tilde{\mathcal{L}}^{(\mathbf{t})} f = \nabla_\alpha [-\tilde{b}^{\mu(\alpha} \nabla_\mu v^{\beta)} f_\beta + v^\mu \nabla_\mu \tilde{b}^{\alpha\beta} f_\beta] + \tilde{b}^{\alpha\beta} f_\beta \nabla_\alpha \nabla_\mu v^\mu.$$

Recall that the divergence of cofactor is zero ($\nabla_\alpha \tilde{b}^{\alpha\mu} = 0$),

$$\tilde{\mathcal{L}}^{(\mathbf{t})} f = -\tilde{b}^{\mu\alpha} \nabla_\alpha [\nabla_\mu v^\beta f_\beta] - \nabla_\alpha [\tilde{b}^{\mu\beta} \nabla_\mu v^\alpha f_\beta] + \nabla_\alpha [v^\mu \nabla_\mu \tilde{b}^{\alpha\beta} f_\beta] + \tilde{b}^{\alpha\beta} f_\beta \nabla_\alpha \nabla_\mu v^\mu$$

$$= -\tilde{b}^{\mu\alpha} \nabla_\alpha [\nabla_\mu (v^\beta f_\beta) - v^\beta \nabla_\mu f_\beta] - \nabla_\alpha [\tilde{b}^{\mu\beta} \nabla_\mu v^\alpha f_\beta] + \nabla_\alpha [v^\mu \nabla_\mu \tilde{b}^{\alpha\beta} f_\beta] + \tilde{b}^{\alpha\beta} f_\beta \nabla_\alpha \nabla_\mu v^\mu$$

$$= -\tilde{b}^{\mu\alpha} \nabla_\alpha \nabla_\mu (f_\beta v^\beta) + \tilde{b}^{\mu\alpha} \nabla_\alpha (v^\beta \nabla_\mu f_\beta) - \tilde{b}^{\mu\beta} f_\beta \nabla_\alpha \nabla_\mu v^\alpha - \nabla_\mu v^\alpha \tilde{b}^{\mu\beta} \nabla_\alpha f_\beta$$
$$- \cancel{\nabla_\mu v^\alpha f_\beta \nabla_\alpha \tilde{b}^{\mu\beta}} + \cancel{\nabla_\alpha v^\mu \nabla_\mu \tilde{b}^{\alpha\beta} f_\beta} + v^\mu \nabla_\alpha [\nabla_\mu \tilde{b}^{\alpha\beta} f_\beta] + \tilde{b}^{\alpha\beta} f_\beta \nabla_\alpha \nabla_\mu v^\mu.$$

Combining the second and fourth term,

$$2^{nd} + 4^{th} = \tilde{b}^{\mu\alpha} v^\beta \nabla_\alpha \nabla_\mu f_\beta + \cancel{\tilde{b}^{\mu\alpha} \nabla_\alpha v^\beta \nabla_\mu f_\beta} - \cancel{\nabla_\mu v^\alpha \tilde{b}^{\mu\beta} \nabla_\alpha f_\beta}.$$

$$\therefore \tilde{\mathcal{L}^{(\mathbf{t})}} f = -\tilde{b}^{\mu\alpha} \nabla_\alpha \nabla_\mu (f_\beta v^\beta) + \tilde{b}^{\mu\alpha} v^\beta \nabla_\alpha \nabla_\mu f_\beta + v^\mu \nabla_\alpha [\nabla_\mu \tilde{b}^{\alpha\beta} f_\beta] + \tilde{v}^{\mu\beta} f_\beta [\nabla_\mu \nabla_\alpha - \nabla_\alpha \nabla_\mu] v^\alpha.$$

Recall that $[\nabla_\mu \nabla_\alpha - \nabla_\alpha \nabla_\mu] v^\alpha = -K g_{\mu\alpha} v^\alpha$,

$$\Rightarrow \tilde{\mathcal{L}^{(\mathbf{t})}} f = -\tilde{b}^{\mu\alpha} \nabla_\alpha \nabla_\mu (f_\beta v^\beta) + \tilde{b}^{\mu\alpha} v^\beta \nabla_\alpha \nabla_\mu f_\beta + + v^\mu \nabla_\alpha [\nabla_\mu \tilde{b}^{\alpha\beta} f_\beta] - \tilde{b}^{\mu\beta} f_\beta K g_{\mu\alpha} v^\alpha$$

$$= \tilde{b}^{\mu\alpha} \nabla_\alpha \nabla_\mu (f_\beta v^\beta) + \tilde{b}^{\mu\alpha} v^\beta \nabla_\alpha \nabla_\beta f_\mu + v^\mu \nabla_\alpha [\nabla_\mu (\tilde{b}^{\alpha\beta} f_\beta) - \tilde{b}^{\alpha\beta} \nabla_\mu f_\beta] - \tilde{b}^{\mu\beta} g_{\mu\alpha} K f_\beta v^\alpha$$

$$= -\tilde{b}^{\mu\alpha} \nabla_\alpha \nabla_\mu (f_\beta v^\beta) + \cancel{\tilde{b}^{\mu\alpha} v^\beta \nabla_\alpha \nabla_\beta f_\mu} + v^\mu \nabla_\alpha \nabla_\mu (\tilde{b}^{\alpha\beta} f_\beta) - \cancel{v^\mu \tilde{b}^{\alpha\beta} \nabla_\alpha \nabla_\mu f_\beta} - \tilde{b}^{\mu\beta} g_{\mu\alpha} K f_\beta v^\alpha.$$

Write the third term as follows,

$$3^{rd} = v^\mu \nabla_\alpha \nabla_\mu (\tilde{b}^{\alpha\beta} f_\beta) = v^\beta \nabla_\alpha \nabla_\beta (\tilde{b}^{\alpha\mu} f_\mu) = v^\beta [\nabla_\beta \nabla_\alpha (\tilde{b}^{\alpha\mu} f_\mu) + \mathcal{R}^\alpha_{.\mu\alpha\beta} \tilde{b}^{\mu\nu} f_\nu]$$

$$= v^\beta \nabla_\beta \nabla_\alpha (\tilde{b}^{\alpha\mu} f_\mu) + v^\beta K g_{\mu\beta} \tilde{b}^{\mu\nu} f_\nu$$

$$= v^\beta \nabla_\beta [\tilde{b}^{\alpha\mu} \nabla_\alpha f_\mu] + v^\alpha K \tilde{b}^{\mu\beta} g_{\mu\alpha} f_\beta.$$

Therefore,

$$\tilde{\mathcal{L}}^{(\mathbf{t})} f = -\tilde{b}^{\mu\alpha} \nabla_\alpha \nabla_\mu (f_\beta v^\beta) + v^\beta \nabla_\beta [\tilde{b}^{\alpha\mu} \nabla_\alpha \nabla_\mu f] + \cancel{v^\alpha K \tilde{b}^{\mu\beta} g_{\mu\alpha} f_\beta} - \cancel{\tilde{b}^{\mu\beta} g_{\mu\alpha} K f_\beta v^\alpha}$$

$$= -\tilde{\Delta}(f_\beta v^\beta) + v^\beta \nabla_\beta [\tilde{\Delta} f].$$

□

Lemma 9.

$$\tilde{\mathcal{L}}^{(n)} f = (\Delta f)(\Delta w) + 2Hw\tilde{\Delta} f - \nabla_{\alpha\beta} f \nabla^{\alpha\beta} w - K \nabla w \cdot \nabla f.$$

Proof. Recall that,

$$\tilde{\mathcal{L}}^{(n)} f = \nabla_\alpha [\tilde{\mathfrak{b}}^{\alpha\beta(n)} \nabla_\beta f] + \tilde{b}^{\alpha\beta} \nabla_\beta f \nabla_\alpha \Big(\frac{\mathfrak{g}^{(n)}}{2g} \Big)$$

$$= \nabla_\alpha \Big[\Big(g^{\alpha\beta} \Delta w + 2H\tilde{b}^{\alpha\beta} w - \nabla^{\alpha\beta} w \Big) \nabla_\beta f \Big] + \tilde{b}^{\alpha\beta} \nabla_\beta f \nabla \Big(-2Hw \Big)$$

$$= \nabla_\alpha \Big[\nabla^\alpha f \Delta w + 2\tilde{b}^{\alpha\beta} H (\nabla_\beta f) w - \nabla_\beta f \nabla^{\alpha\beta} w \Big] - 2\tilde{b}^{\alpha\beta} \nabla_\beta f \nabla_\alpha (Hw)$$

$$= (\Delta f)(\Delta w) + \nabla^\alpha f \nabla_\alpha (\Delta w) + \cancel{2\tilde{b}^{\alpha\beta} (\nabla_\beta f) \nabla_\alpha (Hw)} + 2Hw \nabla_\alpha (\tilde{b}^{\alpha\beta} \nabla_\beta f)$$
$$- \nabla_\alpha \Big[(\nabla_\beta f) \nabla^{\alpha\beta} w \Big] - \cancel{2\tilde{b}^{\alpha\beta} (\nabla_\beta f) \nabla_\alpha (Hw)}.$$

Since, $\tilde{b}^{\alpha\beta}$ is divergence-free and by definition, $\tilde{\Delta} f = \tilde{b}^{\alpha\beta} \nabla_{\alpha\beta} f$, we have,

$$\tilde{\mathcal{L}}^{(n)} f = (\Delta f)(\Delta w) + \nabla^\alpha f \nabla_\alpha (\Delta w) + 2Hw\tilde{\Delta} f - \nabla_\alpha \Big[\nabla_\beta f \nabla^{\alpha\beta} w \Big].$$

We shall now show that the last term in the previous expression can be written as follows,

$$\nabla_\alpha\Big[\nabla_\beta f\nabla^{\alpha\beta}w\Big] = \nabla_{\alpha\beta}f\nabla^{\alpha\beta w} + K\nabla w\cdot\nabla f + \nabla f\cdot\nabla(\Delta w).$$

Consider the left side of the previous equation,

$$\begin{aligned}\nabla_\alpha\Big[\nabla_\beta f\nabla^{\alpha\beta}w\Big] &= \nabla_{\alpha\beta}f\nabla^{\alpha\beta}w + (\nabla_\beta f)\nabla_\alpha\Big(\nabla^\alpha\nabla^\beta w\Big)\\ &= \nabla_{\alpha\beta}f\nabla^{\alpha\beta}w + (\nabla_\beta f)\nabla_\alpha\Big(\nabla^\beta\nabla^\alpha w\Big),\end{aligned}$$

where, the last equality follows from the fact that for scalar function, covariant derivatives commute. Let us write $w^\alpha := \nabla^\alpha w$. Observe the following equation,

$$\Big(\nabla_\alpha\nabla_\beta - \nabla_\beta\nabla_\alpha\Big)w^\gamma = \mathcal{R}^\gamma_{.\delta\alpha\beta}w^\delta.$$

Therefore,

$$\begin{aligned}\Big(\nabla_\alpha\nabla_\beta - \nabla_\beta\nabla_\alpha\Big)w^\alpha &= Kg_{\delta\beta}w^\delta,\\ \Rightarrow \nabla_\alpha\nabla^\beta w^\alpha = Kw^\beta + \nabla^\beta\nabla_\alpha w^\alpha &= Kw^\beta + \nabla^\beta(\Delta w).\end{aligned}$$

With this, it easily follows that

$$\nabla_\alpha\Big[\nabla_\beta f\nabla^{\alpha\beta}w\Big] = \nabla_{\alpha\beta}f\nabla^{\alpha\beta}w + K\nabla w\cdot\nabla f + \nabla f\cdot\nabla(\Delta w).$$

It then follows,

$$\tilde{\mathcal{L}}^{(n)}f = (\Delta f)(\Delta w) + 2Hw\tilde{\Delta}f - \nabla_{\alpha\beta}f\nabla^{\alpha\beta}w - K\nabla w\cdot\nabla f$$

The following lemma immediately follows from the definition of variation of $\tilde{\Delta}c_g$.

Lemma 10.

$$\delta(\tilde{\Delta}c_g) = \tilde{\Delta}[c_g'(\psi + \mathbf{v}\cdot\nabla\phi)] + \tilde{\mathcal{L}}c_g.$$

Proposition 14.

$$\int_\omega w\tilde{\mathcal{L}}^{(n)}c_g'\,da = \int_\omega\Big[\nabla_\beta w\nabla^{\alpha\beta}c_g'\nabla_\alpha w - \Delta(c_g')\nabla w\cdot\nabla w\Big]\,da.$$

□

C.4 Simplifying Second Variation

Recall the second variation,

$$\delta^2\mathcal{E} = \int_\omega \hat{\mathcal{F}}_n w + \hat{\mathcal{F}}_\phi \psi \, da, \tag{C.16}$$

where,

$$\hat{\mathcal{F}}_\phi = \delta[-\epsilon\Delta\phi + W' + c'H^2 + c_g' K\lambda] = -\epsilon(\Delta\psi + \mathcal{L}\phi) + (W'' + c''H^2 + c_g'' K)\psi + 2c'H\delta H + c_g'\delta K + \tau,$$

$$\hat{\mathcal{F}}_n = \left\{\epsilon\mathfrak{b}^{\alpha\beta}\phi_\alpha\phi_\beta + 2\epsilon b^{\alpha\beta}\phi_\alpha\psi_\beta + \delta[\Delta(cH)] + \delta[\tilde{\Delta}c_g] + 2\delta[cH(H^2 - K)] - 2\tilde{\gamma}\delta H - 2H\delta\tilde{\gamma}\right\}.$$

Definition 24.

$$\hat{\mathcal{F}}_\phi =: \hat{\mathcal{F}}_\phi^{(n)} + \hat{\mathcal{F}}_\phi^{(\mathbf{t})} + \hat{\mathcal{F}}_\phi^{(c)} + \hat{\mathcal{F}}_\phi^{(Lag)},$$

$$\hat{\mathcal{F}}_n =: \hat{\mathcal{F}}_n^{(n)} + \hat{\mathcal{F}}_n^{(\mathbf{t})} + \hat{\mathcal{F}}_n^{(c)} + \hat{\mathcal{F}}_n^{(Lag)}.$$

Proposition 15.

$$(a)\, \hat{\mathcal{F}}_\phi^{(c)} = -\epsilon\Delta\psi + (W'' + c''H^2 + c_g'' K)\psi,\ \hat{\mathcal{F}}_\phi^{(Lag)} = \tau,$$

$$(b)\, \hat{\mathcal{F}}_\phi^{(n)} = -2\epsilon\left\{\nabla_\alpha(b^{\alpha\beta}w\phi_\beta) - \nabla^\alpha(Hw)\phi_\alpha\right\} + 2c'H\left[\frac{\Delta w}{2} + (2H^2 - K)w\right] + c_g'[\tilde{b}^{\alpha\beta}\nabla_{\alpha\beta}w + 2KHw],$$

$$(c)\, \hat{\mathcal{F}}_\phi^{(\mathbf{t})} = 0.$$

Proof. (a) is trivial.

(b)

$$\hat{\mathcal{F}}_\phi^{(n)} = -\epsilon\mathcal{L}^{(n)}\phi + 2Hc'\delta^{(n)}H + c_g'\delta^{(n)}K$$

$$= -2\epsilon\left\{\nabla_\alpha(b^{\alpha\beta}w\phi_\beta) - \nabla^\alpha(Hw)\phi_\alpha\right\} + 2c'H\delta^{(n)}H + c_g'\delta^{(n)}K$$

The result follows from the definitions of $\delta^{(n)}H$ and $\delta^{(n)}K$.

(c)

$$\hat{\mathcal{F}}_\phi^{(\mathbf{t})} = -\epsilon\Big(\Delta(\nabla\phi\cdot\mathbf{v}) + \mathcal{L}^{(\mathbf{t})}\phi\Big) + 2c'H\delta^{(\mathbf{t})}H + c_g'\delta^{(\mathbf{t})}K + (W'' + c''H^2 + c_g'' K)(\nabla\phi\cdot\mathbf{v})$$

Using proposition (10) for $\mathcal{L}^{(\mathbf{t})}\phi$,

$$-\epsilon\mathcal{L}^{(\mathbf{t})}\phi+2c'H\delta^{(\mathbf{t})}H+c'_g\delta^{(\mathbf{t})}K=\epsilon\left\{\Delta v^\beta\phi_\beta+\phi_\beta v^\beta K+2\nabla^\alpha v^\beta\nabla_{\alpha\beta}\phi\right\}+2c'H\nabla H\cdot\mathbf{v}+c'_g\nabla K\cdot\mathbf{v}$$

$$=\epsilon\left\{\nabla_\alpha\nabla^\alpha v^\beta\phi_\beta+2\nabla^\alpha v^\beta\nabla_\alpha\phi_\beta+\phi_\beta v^\beta K\right\}+c'\nabla H^2\cdot\mathbf{v}+c'_g\nabla K\cdot\mathbf{v}$$

$$=\epsilon\left\{\nabla_\alpha[\nabla^\alpha v^\beta\phi_\beta]+\nabla^\alpha v^\beta\nabla_\alpha\phi_\beta+\phi_\beta v^\beta K\right\}+c'\nabla H^2\cdot\mathbf{v}+c'_g\nabla K\cdot\mathbf{v}$$

$$=\epsilon\left\{\nabla_\alpha[\nabla^\alpha(v^\beta\phi_\beta)-v^\beta\nabla^\alpha\phi_\beta]+\nabla^\alpha v^\beta\nabla_\alpha\phi_\beta+\phi_\beta v^\beta K\right\}+c'\nabla H^2\cdot\mathbf{v}+c'_g\nabla K\cdot\mathbf{v}$$

$$=\epsilon\left\{\Delta(\phi_\beta v^\beta)-\nabla_\alpha(v^\beta\nabla^\alpha\phi_\beta)+\nabla^\alpha v^\beta\nabla_\alpha\phi_\beta+\phi_\beta v^\beta K\right\}+c'\nabla H^2\cdot\mathbf{v}+c'_g\nabla K\cdot\mathbf{v}$$

$$=\epsilon\left\{\Delta(\phi_\beta v^\beta)-v^\beta\Delta\phi_\beta+\phi_\beta v^\beta K\right\}+c'\nabla H^2\cdot\mathbf{v}+c'_g\nabla K\cdot\mathbf{v}$$

Using proposition (11), $\Delta\phi_\beta=\nabla_\beta(\Delta\phi)+K\phi_\beta$,

$$-\epsilon\mathcal{L}^{(\mathbf{t})}\phi+2c'H\delta^{(\mathbf{t})}H+c'_g\delta^{(\mathbf{t})}K=\epsilon\left\{\Delta(\phi_\beta v^\beta)-v^\beta\nabla_\beta(\Delta\phi)\right\}.$$

Using the equilibrium concentration equation, $\epsilon\Delta\phi=W'+\lambda+c'H^2+c'_gK$,

$$-\epsilon\mathcal{L}^{(\mathbf{t})}\phi+2c'H\delta^{(\mathbf{t})}H+c'_g\delta^{(\mathbf{t})}K=\epsilon\Delta(\phi_\beta v^\beta)-(W''+c''H^2+c''_gK)\phi_\beta v^\beta.$$

Substituting this in the expression for $\hat{\mathcal{F}}^{(\mathbf{t})}_\phi$, we conclude that

$$\hat{\mathcal{F}}^{(\mathbf{t})}_\phi=0.$$

□

We now establish the following important theorem.

Theorem 8.

$$\hat{\mathcal{F}}^{(\mathbf{t})}_n=0.$$

The following lemmas are in order.

Lemma 11.

$$\delta^{(\mathbf{t})}[\Delta(cH)]=v^\alpha\nabla_\alpha[\Delta(cH)].$$

Proof. Let us first note that,

$$\delta^{(\mathbf{t})}(cH) = (Hc'\nabla\phi + c\nabla H)\cdot\mathbf{v} = \nabla(cH)\cdot\mathbf{v}.$$

So,

$$\delta^{(\mathbf{t})}\Delta(cH) = \Delta[\delta^{(\mathbf{t})}(cH)] + \mathcal{L}^{(\mathbf{t})}(cH).$$

$$= \Delta((cH)_\alpha v^\alpha) - \Delta v^\alpha (cH)_\alpha - (cH)_\alpha v^\alpha K - 2\nabla^\alpha v^\beta \nabla_{\alpha\beta}(cH). \tag{C.17}$$

Since,

$$\Delta((cH)_\alpha v^\alpha) = \nabla^\beta\nabla_\beta((cH)_\alpha v^\alpha) = \nabla^\beta[\nabla_\beta(cH)_\alpha v^\alpha + (cH)_\alpha \nabla_\beta v^\alpha]$$

$$= \nabla^\beta\nabla_\beta((cH)_\alpha)v^\alpha + \nabla_{\alpha\beta}(cH)\nabla^\beta v^\alpha + \nabla^\beta\nabla_\alpha(cH)\nabla_\beta v^\alpha + \nabla_\alpha(cH)\Delta v^\alpha$$

$$= \Delta((cH)_\alpha)v^\alpha + 2\nabla^\beta v^\alpha \nabla_{\alpha\beta}(cH) + \nabla_\alpha(cH)\Delta v^\alpha.$$

The last two terms get cancelled as they appear with the opposite signs in the original expression in equation (C.17), which then reduces to

$$\Delta(\delta^{(\mathbf{t})}(cH)) + \mathcal{L}^{(\mathbf{t})}cH = \Delta((cH)_\alpha)v^\alpha - \nabla_\alpha(cH)v^\alpha K$$

Now, by using proposition (11), the last term above gets cancelled and we have

$$\Delta(\delta^{(\mathbf{t})}(cH)) + \mathcal{L}^{(\mathbf{t})}cH = v^\alpha\nabla_\alpha(\Delta(cH)).$$

□

Lemma 12.

$$\hat{\mathcal{F}}_n^{(\mathbf{t})} = \epsilon\left\{2H\nabla^\beta(\phi_\alpha\phi_\beta v^\alpha) - v^\alpha\nabla_\alpha(b^{\mu\nu}\phi_\mu\phi_\nu) + \mathfrak{b}^{(\mathbf{t})\alpha\beta}\phi_\alpha\phi_\beta\right\} + 2\epsilon\Big[b^{\alpha\beta}\phi_\alpha(\nabla\phi\cdot\mathbf{v})_\beta - H(\phi^\alpha\nabla\phi\cdot\mathbf{v})_\alpha\Big].$$

Proof.

$$\hat{\mathcal{F}}_n^{(\mathbf{t})} = \Big\{\epsilon\mathfrak{b}^{(\mathbf{t})\alpha\beta}\phi_\alpha\phi_\beta + 2\epsilon b^{\alpha\beta}\phi_\alpha(\nabla\phi\cdot\mathbf{v})_\beta + \delta^{(\mathbf{t})}\Delta(cH) + 2\delta^{(\mathbf{t})}[cH(H^2-K)] \\ -2\delta^{(\mathbf{t})}H\tilde{\gamma} - 2H\delta^{(\mathbf{t})}\tilde{\gamma} + \delta^{(\mathbf{t})}\tilde{\Delta}c_g\Big\} \quad \text{(C.18)}$$

By using lemma (11), we have

$$\delta^{(\mathbf{t})}\Delta(cH) = v^\alpha\nabla_\alpha\Delta(cH),$$

and using the facts that $\delta^{(\mathbf{t})}H = v^\alpha\nabla_\alpha H$, $\delta^{(\mathbf{t})}K = v^\alpha\nabla_\alpha K$ and $\delta^{(\mathbf{t})}c = \nabla c\cdot\mathbf{v}$,

$$\delta^{(\mathbf{t})}[cH(H^2-K)] = v^\alpha\nabla_\alpha[cH(H^2-K)].$$

Let's now write,

$$-2\delta^{(\mathbf{t})}H\tilde{\gamma} = -2v^\alpha\tilde{\gamma}\nabla_\alpha H$$

$$= -2v^\alpha\nabla_\alpha(H\tilde{\gamma}) + 2v^\alpha H\nabla_\alpha\tilde{\gamma}.$$

We write,

$$\nabla_\alpha\tilde{\gamma} = (W'+\lambda)\nabla_\alpha\phi + \frac{\epsilon}{2}\nabla_\alpha|\nabla\phi|^2.$$

Using the concentration equilibrium equation, (2.30b) and proposition (1), we have

$$\nabla_\alpha\tilde{\gamma} = \epsilon\nabla^\beta(\phi_\alpha\phi_\beta) - (c'H^2 + c'_gK)\nabla_\alpha\phi.$$

We then have,

$$-2\delta^{(\mathbf{t})}H\tilde{\gamma} = -2v^\alpha\nabla_\alpha(H\tilde{\gamma}) + 2\epsilon v^\alpha H\nabla^\beta(\phi_\alpha\phi_\beta) - 2(c'H^2 + c'_gK)(\nabla_\alpha\phi)Hv^\alpha.$$

Note that,

$$\delta^{(\mathbf{t})}\tilde{\gamma} = (W'+\lambda)\nabla\phi\cdot\mathbf{v} + \frac{\epsilon}{2}\Big[\mathfrak{g}^{\alpha\beta}\phi_\alpha\phi_\beta + 2g^{\alpha\beta}\phi_\alpha(\nabla\phi\cdot\mathbf{v})_\beta\Big].$$

Furthermore,

$$\delta^{(\mathbf{t})}(\tilde{\Delta}c_g) = v^\alpha\nabla_\alpha(\tilde{\Delta}c_g)$$

Using the above facts, we can then write,

$$\hat{\mathcal{F}}_n^{(\mathbf{t})} = \Big\{\epsilon\mathfrak{b}^{(\mathbf{t})\alpha\beta}\phi_\alpha\phi_\beta + v^\alpha\nabla_\alpha[\tilde{\Delta}c_g + \Delta(cH) + 2cH(H^2-K) - 2\tilde{\gamma}H - p] \\ +2\epsilon v^\alpha H\nabla^\beta(\phi_\alpha\phi_\beta) - \epsilon H\mathfrak{g}^{(\mathbf{t})\alpha\beta}\phi_\alpha\phi_\beta\Big\}$$

If we now use the normal equilibrium equation, we can replace the second term above by $-\epsilon v^\alpha\nabla_\alpha[b^{\mu\nu}\phi_\mu\phi_\nu]$

$$\hat{\mathcal{F}}_n^{(\mathbf{t})} = \epsilon\left\{[\mathfrak{b}^{(\mathbf{t})\alpha\beta} - H\mathfrak{g}^{(\mathbf{t})\alpha\beta}]\phi_\alpha\phi_\beta - v^\alpha\nabla_\alpha(b^{\mu\nu}\phi_\mu\phi_\nu) + 2v^\alpha H\nabla^\beta(\phi_\alpha\phi_\beta)\right\}$$

Since $-\mathfrak{g}^{(\mathbf{t})\alpha\beta}\phi_\alpha\phi_\beta = 2\nabla^\beta v^\alpha\phi_\alpha\phi_\beta$,

$$\hat{\mathcal{F}}_n^{(\mathbf{t})} = \epsilon\left\{\mathfrak{b}^{(\mathbf{t})\alpha\beta}\phi_\alpha\phi_\beta - v^\alpha\nabla_\alpha(b^{\mu\nu}\phi_\mu\phi_\nu) + 2H\nabla^\beta(\phi_\alpha\phi_\beta v^\alpha)\right\}$$

□

Lemma 13.

$$\mathfrak{b}^{\alpha\beta}\phi_\alpha\phi_\beta = \phi^\mu\phi^\nu\mathfrak{b}_{\mu\nu} + 2\phi_\alpha\phi_\beta b_\mu^\beta[-\nabla^{(\alpha}v^{\mu)} + 2b^{\alpha\mu}w]$$

Proof.

$$b^{\alpha\beta} = g^{\alpha\mu}g^{\beta\nu}b_{\mu\nu}$$

$$\delta b^{\alpha\beta} = \delta(g^{\alpha\mu}g^{\beta\nu}b_{\mu\nu})$$

$$= \mathfrak{g}^{\alpha\mu}b_\mu^\beta + \mathfrak{g}^{\beta\nu}b_\nu^\alpha + g^{\alpha\mu}g^{\beta\nu}\mathfrak{b}_{\mu\nu}$$

$$\Rightarrow \mathfrak{b}^{\alpha\beta}\phi_\alpha\phi_\beta = 2\phi_\alpha\phi_\beta b_\mu^\beta\mathfrak{g}^{\alpha\mu} + \phi^\mu\phi^\nu\mathfrak{b}_{\mu\nu}$$

The result now follows using the fact that $\mathfrak{g}^{\alpha\mu} = -\nabla^{(\alpha}v^{\mu)} + 2b^{\alpha\mu}w$. □

Proof. (Theorem) Using Lemma (12),

$$\hat{\mathcal{F}}_n^{(\mathbf{t})} = \epsilon\left\{2H\nabla^\beta(\phi_\alpha\phi_\beta v^\alpha) - v^\alpha\nabla_\alpha(b^{\mu\nu}\phi_\mu\phi_\nu) + \mathfrak{b}^{(\mathbf{t})\alpha\beta}\phi_\alpha\phi_\beta\right\}$$

$$= \epsilon \left\{ 2H\nabla^{\beta}(\phi_{\alpha}\phi_{\beta}v^{\alpha}) - v^{\alpha}\nabla_{\alpha}(b^{\mu\nu}\phi_{\mu}\phi_{\nu}) + \mathfrak{b}^{(\mathbf{t})\alpha\beta}\phi_{\alpha}\phi_{\beta} \right\} \tag{C.19}$$

Recall that

$$\mathfrak{b}^{(\mathbf{t})}_{\alpha\beta} = \nabla_{\alpha}v^{\mu}b_{\mu\beta} + \nabla_{\beta}(v^{\mu}b_{\mu\alpha})$$

$$\Rightarrow \phi^{\alpha}\phi^{\beta}\mathfrak{b}^{(\mathbf{t})}_{\alpha\beta} = \phi^{\alpha}\phi^{\beta}[\nabla_{\alpha}v^{\mu}b_{\mu\beta} + \nabla_{\beta}(v^{\mu}b_{\mu\alpha})]$$

$$= \phi^{\alpha}\phi^{\beta}\nabla_{\alpha}v^{\mu}b_{\mu\beta} + \phi^{\alpha}\phi^{\beta}\nabla_{\beta}v^{\mu}b_{\mu\alpha} + \phi^{\alpha}\phi^{\beta}v^{\mu}\nabla_{\beta}b_{\mu\alpha}$$

$$= 2\phi^{\alpha}\phi^{\beta}\nabla_{\alpha}v^{\mu}b_{\mu\beta} + \phi^{\alpha}\phi^{\beta}v^{\mu}\nabla_{\beta}b_{\mu\alpha}$$

Now,

$$\mathfrak{b}^{(\mathbf{t})\alpha\beta}\phi_{\alpha}\phi_{\beta} = \phi^{\alpha}\phi^{\beta}\mathfrak{b}^{(\mathbf{t})}_{\alpha\beta} - 2\phi_{\alpha}\phi_{\beta}b^{\beta}_{\mu}\nabla^{(\alpha}v^{\mu)}$$

$$= 2\phi^{\alpha}\phi^{\beta}\nabla_{\alpha}v^{\mu}b_{\mu\beta} + \phi^{\alpha}\phi^{\beta}v^{\mu}\nabla_{\beta}b_{\mu\alpha} - 2\phi_{\alpha}\phi_{\beta}b^{\beta}_{\mu}\nabla^{(\alpha}v^{\mu)}$$

$$= -2\phi_{\alpha}\phi_{\beta}b^{\beta}_{\mu}\nabla^{\mu}v^{\alpha} + \phi^{\alpha}\phi^{\beta}v^{\mu}\nabla_{\beta}b_{\mu\alpha}$$

Expanding the second term in Eq. (C.19),

$$-v^{\mu}\nabla_{\mu}(b^{\alpha\beta}\phi_{\alpha}\phi_{\beta}) = -v^{\mu}\nabla_{\mu}b^{\alpha\beta}\phi_{\alpha}\phi_{\beta} - v^{\mu}b^{\alpha\beta}\nabla_{\mu}(\phi_{\alpha}\phi_{\beta})$$

$$= -v^{\mu}\nabla_{\mu}b_{\alpha\beta}\phi^{\alpha}\phi^{\beta} - v^{\mu}b^{\alpha\beta}\nabla_{\mu}(\phi_{\alpha}\phi_{\beta})$$

$$= -v^{\mu}\nabla_{\beta}b_{\alpha\mu}\phi^{\alpha}\phi^{\beta} - v^{\mu}b^{\alpha\beta}\nabla_{\mu}(\phi_{\alpha}\phi_{\beta})$$

Where the last line follows from Codazzi-Mainardi Equations. We then have,

$$-v^{\mu}\nabla_{\mu}(b^{\alpha\beta}\phi_{\alpha}\phi_{\beta}) + \mathfrak{b}^{(\mathbf{t})\alpha\beta}\phi_{\alpha}\phi_{\beta} = -2\phi_{\alpha}\phi_{\beta}b^{\beta}_{\mu}\nabla^{\mu}v^{\alpha} - v^{\mu}b^{\alpha\beta}\nabla_{\mu}(\phi_{\alpha}\phi_{\beta})$$

$$\hat{\mathcal{F}}^{(\mathbf{t})}_{n} = \epsilon \left\{ 2H\nabla^{\beta}(\phi_{\alpha}v^{\alpha}\phi_{\beta}) - 2\phi_{\alpha}\phi_{\beta}b^{\beta}_{\mu}\nabla^{\mu}v^{\alpha} - v^{\mu}b^{\alpha\beta}\nabla_{\mu}(\phi_{\alpha}\phi_{\beta}) \right\}$$

$$\hat{\mathcal{F}}^{(\mathbf{t})}_{n} = \epsilon \left\{ 2H\nabla^{\beta}(\phi_{\alpha}v^{\alpha}\phi_{\beta}) - 2\phi_{\alpha}\phi_{\beta}b^{\beta}_{\mu}\nabla^{\mu}v^{\alpha} - 2v^{\mu}b^{\alpha\beta}\phi_{\beta}\nabla_{\mu}(\phi_{\alpha}) \right\}$$

$(\mu \to \alpha, \alpha \to \mu)$ in the third term above,

$$\hat{\mathcal{F}}^{(\mathbf{t})}_{n} = \epsilon \left\{ 2H\nabla^{\beta}(\phi_{\alpha}v^{\alpha}\phi_{\beta}) - 2\phi_{\alpha}\phi_{\beta}b^{\beta}_{\mu}\nabla^{\mu}v^{\alpha} - 2v^{\alpha}b^{\mu\beta}\phi_{\beta}\nabla_{\alpha}\phi_{\mu} \right\}$$

Now, using the fact that, $\nabla_\mu \phi_\alpha = \nabla_\alpha \phi_\mu = \nabla_{\alpha\mu}\phi$,

$$\hat{\mathcal{F}}_n^{(\mathbf{t})} = \epsilon \left\{ 2H\nabla^\beta(\phi_\alpha v^\alpha \phi_\beta) - 2\phi_\alpha \phi_\beta b^{\beta\mu} \nabla_\mu v^\alpha - 2v^\alpha b^{\mu\beta}\phi_\beta \nabla_\mu \phi_\alpha \right\}$$

$$= \epsilon \left\{ 2H\nabla^\beta(\phi_\alpha v^\alpha \phi_\beta) - b^{\beta\mu}\phi_\beta \nabla_\mu(\phi_\alpha v^\alpha) \right\}$$

Therefore,

$$\int_\omega w\hat{\mathcal{F}}_n^{(\mathbf{t})} = \epsilon \int_\omega 2w \left\{ H\nabla^\beta(\phi_\alpha v^\alpha \phi_\beta) - b^{\beta\mu}\phi_\beta \nabla_\mu(\phi_\alpha v^\alpha) \right\}$$

$$= \epsilon \int_\omega -2\nabla^\beta(wH)\phi_\beta \phi_\alpha v^\alpha + 2\nabla_\mu(b^{\beta\mu} w\phi_\beta)\phi_\alpha v^\alpha \text{ (IBP)}$$

$$= \int_\omega 2\epsilon \left\{ \nabla_\mu(b^{\beta\mu} w\phi_\beta) - \nabla_\beta(wH)\phi^\beta \right\} \nabla\phi \cdot \mathbf{v}$$

$$= -\int_\omega \hat{\mathcal{F}}_\phi^{(n)} \nabla\phi \cdot \mathbf{v}$$

□

Theorem 9.

$$\int_\omega w\hat{\mathcal{F}}_n^{(\psi)} = \int_\omega \psi \hat{\mathcal{F}}_\phi^{(n)}$$

Proof.

$$\hat{\mathcal{F}}_n^{(\psi)} = 2\epsilon b^{\alpha\beta}\phi_\alpha \psi_\beta - 2H[W'\psi + \epsilon g^{\alpha\beta}\phi_\alpha \psi_\beta + \lambda\psi]$$

$$\int_\omega w\hat{\mathcal{F}}_n^{(\psi)} = \int_\omega \left\{ 2w\epsilon b^{\alpha\beta}\phi_\alpha \psi_\beta - 2Hw[(W' + \lambda)\psi + \epsilon g^{\alpha\beta}\phi_\alpha \psi_\beta] \right\}$$

$$= \int_\omega -2\epsilon\nabla_\beta(b^{\alpha\beta} w\phi_\alpha)\psi + 2\epsilon\nabla_\beta(Hwg^{\alpha\beta}\phi_\alpha)\psi - 2Hw(W' + \lambda)\psi \text{ (IBP)}$$

$$= \int_\omega -2\epsilon\nabla_\beta(b^{\alpha\beta} w\phi_\alpha)\psi + 2\epsilon\nabla_\beta(Hw)\phi^\beta\psi + 2\epsilon\nabla_\beta(\phi^\beta)Hw\psi - 2Hw(W' + \lambda)\psi$$

$$= \int_\omega -2\epsilon\nabla_\beta(b^{\alpha\beta} w\phi_\alpha)\psi + 2\epsilon\nabla_\beta(Hw)\phi^\beta\psi + 2[\epsilon\Delta\phi - (W' + \lambda)]Hw\psi$$

The last term falls out due to Concentration equilibrium, $\mathcal{F}_\phi = 0$. Therefore,

$$\int_\omega w\hat{\mathcal{F}}_n^{(\psi)} = \int_\omega \hat{\mathcal{F}}_\phi^{(n)}\psi$$

□

The following proposition is obvious to see.

Proposition 16.

$$\hat{\mathcal{F}}_n^{(Lag)} = -2H[\sigma + \tau(\phi - \mu)]$$

The following Corollary follows as a consequence of the above two theorems.

Corollary 5.

$$\int_\omega w\left(\hat{\mathcal{F}}_n^{(\mathbf{t})} + \hat{\mathcal{F}}_n^{(\psi)}\right) = \int_\omega \hat{\mathcal{F}}_\phi^{(n)}\left(\psi - \nabla\phi\cdot\mathbf{v}\right)$$

With all the results above, we can write the second variation as follows

$$\delta^2\mathcal{E} = \int_\omega \hat{\mathcal{F}}_n w + \hat{\mathcal{F}}_\phi \psi\, da$$

$$= \int_\omega \hat{\mathcal{F}}_n^{(n)} w + \left(2\hat{\mathcal{F}}_\phi^{(n)} + \mathcal{L}^{CH}[\psi]\right)\psi$$

where, $\mathcal{L}^{CH}\cdot = -\epsilon\Delta(\cdot) + W''\cdot$ and the variations w and ψ satisfy

$$\int_\omega Hw\, da = 0 \tag{C.20}$$

$$\int_\omega [\psi - 2H\phi w]\, da = 0 \tag{C.21}$$

C.5 Computing $\int w\hat{\mathcal{F}}_n^{(n)}$

Proposition 17.

$$\int_\omega w\delta^{(n)}(\Delta H) = \int_\omega \frac{1}{2}(\Delta w)^2 + w(2H^2 - K)\Delta w + 2w[H\nabla^\alpha H - b^{\alpha\beta}\nabla_\beta H]\nabla_\alpha w$$
$$+ 2Hw^2\Delta H$$

Proof.

$$\begin{aligned}\int w\delta^{(n)}(\Delta H) &= \int w[\Delta(\delta^{(n)}H) + \mathcal{L}^{(n)}H] \\ &= \int w\left\{\Delta[\frac{\Delta}{2}w + (2H^2 - K)w] + 2\nabla_\alpha(b^{\alpha\beta}wH_\beta) - 2\nabla_\alpha(Hw)\nabla^\alpha H\right\} \\ &= (\text{IBP})\int \frac{(\Delta w)^2}{2} + (2H^2 - K)w\Delta w - 2b^{\alpha\beta}H_\beta w\nabla_\alpha w + 2Hw\nabla_\alpha(w\nabla^\alpha H) \\ &= \int \frac{(\Delta w)^2}{2} + (2H^2 - K)w\Delta w - 2b^{\alpha\beta}H_\beta w\nabla_\alpha w + 2Hw^2\Delta H + 2Hw\nabla^\alpha H\nabla_\alpha w \\ &= \int \frac{(\Delta w)^2}{2} + (2H^2 - K)w\Delta w - 2b^{\alpha\beta}H_\beta w\nabla_\alpha w + 2Hw^2\Delta H + 2Hw\nabla_\alpha w\nabla^\alpha H\end{aligned}$$

□

Proposition 18.

$$-\int_\omega 2\tilde{\gamma}\delta^{(n)}Hw = \int_\omega -\tilde{\gamma}w\Delta w + 2\tilde{\gamma}Kw^2 - 2H\tilde{\gamma}(2Hw^2)$$

Proof.

$$\begin{aligned}-\int 2\tilde{\gamma}\delta^{(n)}Hw &= \int -2\tilde{\gamma}[\frac{\Delta w}{2} + (2H^2 - K)w]w \\ &= \int -\tilde{\gamma}(w\Delta w) + 2\tilde{\gamma}Kw^2 - 2H\tilde{\gamma}(2Hw^2)\end{aligned}$$

□

Proposition 19.

$$\begin{aligned}\int_\omega w2\delta^{(n)}[H(H^2 - K)] = \int_\omega &(3H^2 - K)w\Delta w + (2Hw^2)[2H(H^2 - K)] - \\ &2H\tilde{b}^{\alpha\beta}w\nabla_{\alpha\beta}w + (8H^4 - 10H^2K + 2K^2)w^2\end{aligned}$$

Proof.

$$
\begin{aligned}
2\delta^{(n)}[H^3 - HK] &= (6H^2 - 2K)\delta^{(n)}H - 2H\delta^{(n)}K \\
&= 2(3H^2 - K)\left[\frac{\Delta w}{2} + (2H^2 - K)w\right] - 2H\left[\tilde{b}^{\alpha\beta}\nabla_{\alpha\beta}w + 2KHw\right] \\
&= (3H^2 - K)\Delta w + 2(3H^2 - K)(2H^2 - K)w - 4H^2Kw - 2H\tilde{b}^{\alpha\beta}\nabla_{\alpha\beta}w \\
&= (3H^2 - K)\Delta w + (12H^4 - 14H^2K + 2K^2)w - 2H\tilde{b}^{\alpha\beta}\nabla_{\alpha\beta}w \\
&= (3H^2 - K)\Delta w + (2Hw)[2H(H^2 - K)] - 2H\tilde{b}^{\alpha\beta}\nabla_{\alpha\beta}w + (8H^4 - 10H^2K + 2K^2)w
\end{aligned}
$$

□

Proposition 20.

$$
\int_\omega \epsilon[\mathfrak{b}^{(n)\alpha\beta} - H\mathfrak{g}^{(n)\alpha\beta}]\phi_\alpha\phi_\beta w = \int_\omega 4\epsilon H w^2 b^{\alpha\beta}\phi_\alpha\phi_\beta + \epsilon\phi^\alpha\phi^\beta w\nabla_{\alpha\beta}w - 3\epsilon K w^2\phi_\alpha\phi^\alpha
$$

Proof.

$$
\begin{aligned}
\mathfrak{b}^{(n)\alpha\beta}\phi_\alpha\phi_\beta &= 2\phi_\alpha\phi_\beta b^\beta_\mu(2b^{\alpha\mu}w) + \phi^\alpha\phi^\beta\mathfrak{b}^{(n)}_{\alpha\beta} = 4\phi_\alpha\phi_\beta b^\beta_\mu b^{\alpha\mu}w + \phi^\alpha\phi^\beta\mathfrak{b}^{(n)}_{\alpha\beta} \\
&= 4\phi_\alpha\phi_\beta b^\beta_\mu b^{\alpha\mu}w + \phi^\alpha\phi^\beta[-wb^\mu_\alpha b_{\mu\beta} + \nabla_{\alpha\beta}w] \\
&= 3\phi_\alpha\phi_\beta b^\beta_\mu b^{\alpha\mu}w + \phi^\alpha\phi^\beta\nabla_{\alpha\beta}w
\end{aligned}
$$

$$
-H\mathfrak{g}^{(n)\alpha\beta}\phi_\alpha\phi_\beta = -2Hb^{\alpha\beta}w\phi_\alpha\phi_\beta
$$

By Cayley-Hamilton, we have $b^{\alpha\mu}b^\beta_\mu = 2Hb^{\alpha\beta} - Kg^{\alpha\beta}$, therefore,

$$
3\phi_\alpha\phi_\beta w b^{\alpha\mu}b^\beta_\mu = 6Hwb^{\alpha\beta}\phi_\alpha\phi_\beta - 3Kw\phi_\alpha\phi^\alpha
$$

Hence,

$$
[\mathfrak{b}^{(n)\alpha\beta} - H\mathfrak{g}^{(n)\alpha\beta}]\phi_\alpha\phi_\beta = 4Hwb^{\alpha\beta}\phi_\alpha\phi_\beta + \phi^\alpha\phi^\beta\nabla_{\alpha\beta}w - 3Kw\phi_\alpha\phi^\alpha
$$

□

Theorem 10.

$$\int_\omega w\hat{\mathcal{F}}_n^{(n)} = \int_\omega \frac{c}{2}(\Delta w)^2 - \left\{[c(H^2-2K)-\tilde{\gamma}]g^{\alpha\beta} + \epsilon\phi^\alpha\phi^\beta + 2Hb^{\alpha\beta}\right\}\nabla_\alpha w\nabla_\beta w$$
$$+\left\{2K\tilde{\gamma} + c[8H^4 - 10H^2K + 2K^2 + 2H\Delta H + 2b^{\alpha\beta}\nabla_{\alpha\beta}H + 6H_\alpha H^\alpha - \Delta K] + \right.$$
$$\left. 2\epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta H - 3K\epsilon\phi^\alpha\phi_\alpha + 2pH\right\}w^2$$

Proof. By the previous three propositions, we have

$$\int w\hat{\mathcal{F}}_n^{(n)} = \int \frac{c}{2}(\Delta w)^2 + [c(5H^2-2K)-\tilde{\gamma}]w\Delta w +$$
$$[\epsilon\phi^\alpha\phi^\beta - 2Hc\tilde{b}^{\alpha\beta}]w\nabla_{\alpha\beta}w + 2c[H\nabla^\alpha H - b^{\alpha\beta}\nabla_\beta H]w\nabla_\alpha w +$$
$$+\{2\tilde{\gamma}K + c[8H^4 - 10H^2K + 2K^2] + 2\epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta H - 3K\epsilon\phi^\alpha\phi_\alpha\}w^2 +$$
$$2Hw^2[\epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta + c\Delta H + 2cH(H^2-K) - 2H\tilde{\gamma}]_p$$

If we now use the fact that $\tilde{b}^{\alpha\beta} = b^{\alpha\beta} - 2Hg^{\alpha\beta}$ in the third term, then $-2Hg^{\alpha\beta}\nabla_{\alpha\beta}w = -2H\Delta w$ which with the factor of $2H$ in front gives a total of $-4H^2\Delta w$. We can thus reduce the $5H^2$ to H^2 in the second term. Thus, we have

$$\int_\omega w\hat{\mathcal{F}}_n^{(n)} = \int_\omega \frac{c}{2}(\Delta w)^2 + [c(H^2-2K)-\tilde{\gamma}]w\Delta w + [\epsilon\phi^\alpha\phi^\beta + 2Hcb^{\alpha\beta}]w\nabla_{\alpha\beta}w$$
$$+ 2c[H\nabla^\alpha H - b^{\alpha\beta}\nabla_\beta H]w\nabla_\alpha w + \left\{2\tilde{\gamma}K + c[8H^4 - 10H^2K + 2K^2]\right.$$
$$\left. +2\epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta H - 3K\epsilon\phi^\alpha\phi_\alpha + 2pH\right\}w^2$$

$$= (IBP)\int \frac{c}{2}(\Delta w)^2 - \{\nabla^\alpha[c(H^2-2K)] - \nabla_\alpha\tilde{\gamma} + \epsilon\nabla_\beta(\phi^\alpha\phi^\beta) + 2c\nabla_\beta(Hb^{\alpha\beta})\}w\nabla_\alpha w +$$
$$2c[H\nabla^\alpha H - b^{\alpha\beta}\nabla_\beta H]w\nabla_\alpha - \{[c(H^2-2K)-\tilde{\gamma}]g^{\alpha\beta} + \epsilon\phi^\alpha\phi^\beta + 2Hcb^{\alpha\beta}\}\nabla_\alpha w\nabla_\beta w +$$
$$\{2\tilde{\gamma}K + c[8H^2 - 10H^2K + 2K^2] + 2\epsilon b^{\alpha\beta}\phi_\alpha\phi_\beta H - 3K\epsilon\phi^\alpha\phi_\alpha + 2pH\}w^2$$

Consider the 2nd and 3rd terms,

$$-\left\{\nabla^\alpha[c(H^2-2K)-\tilde{\gamma}] + \nabla_\beta[\epsilon\phi^\alpha\phi^\beta + 2Hcb^{\alpha\beta}] - 2c[H\nabla^\alpha H - b^{\alpha\beta}\nabla_\beta H]\right\}w\nabla_\alpha w$$

If we now use the tangential equilibrium equation $\epsilon\nabla_\beta(\phi^\alpha\phi^\beta) - \nabla^\alpha\tilde{\gamma} = 0$, we have

$$-\left\{c\nabla^\alpha(H^2 - 2K) + 2c\nabla_\beta(Hb^{\alpha\beta}) - 2cH\nabla^\alpha H + 2cb^{\alpha\beta}\nabla_\beta H\right\} w\nabla_\alpha w$$

$$= 2c\left\{\nabla^\alpha K - 2b^{\alpha\beta}\nabla_\beta H - 2H\nabla^\alpha H\right\} w\nabla_\alpha w$$

where, we have used the Codazzi-Mainardi equation $\nabla_\beta b^{\alpha\beta} = \nabla^\alpha b^\beta_\beta = 2\nabla^\alpha H$

The result follows by combining all the previous terms. □

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